```
=> d his

     (FILE 'HOME' ENTERED AT 15:59:32 ON 07 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 15:59:43 ON 07 AUG 2007
L1             STRUCTURE UPLOADED
L2           0 S L1 SSS SAM
L3           0 S L1 SSS FULL
L4             STRUCTURE UPLOADED
L5           1 S L4 SSS SAM
L6          38 S L4 SSS FULL
L7             STRUCTURE UPLOADED
L8           1 S L7 SSS SAM
L9           3 S L7 SSS FULL
L10            STRUCTURE UPLOADED
L11          0 S L10 SSS SAM
L12          2 S L10 SSS FULL

     FILE 'CAPLUS, MEDLINE' ENTERED AT 16:14:36 ON 07 AUG 2007
L13         21 S L6
L14          1 S L13 AND SKIN
L15         20 S L13 NOT L14
L16          0 S L15 AND WRINKL?
L17          0 S L15 AND WHITEN?
L18          0 S L15 AND ACNE?
L19          0 S L15 AND SILICONE
L20          0 S L15 AND CUTANEOUS?
L21          0 S L15 AND ACCELERAT?
L22          1 S L9
L23          4 S L12
```

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=> d his

     (FILE 'HOME' ENTERED AT 15:59:32 ON 07 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 15:59:43 ON 07 AUG 2007
L1                STRUCTURE UPLOADED
L2             0 S L1 SSS SAM
L3             0 S L1 SSS FULL
L4                STRUCTURE UPLOADED
L5             1 S L4 SSS SAM
L6            38 S L4 SSS FULL
L7                STRUCTURE UPLOADED
L8             1 S L7 SSS SAM
L9             3 S L7 SSS FULL
L10               STRUCTURE UPLOADED
L11            0 S L10 SSS SAM
L12            2 S L10 SSS FULL

     FILE 'CAPLUS, MEDLINE' ENTERED AT 16:14:36 ON 07 AUG 2007
L13           21 S L6
L14            1 S L13 AND SKIN
L15           20 S L13 NOT L14
L16            0 S L15 AND WRINKL?
L17            0 S L15 AND WHITEN?
L18            0 S L15 AND ACNE?
L19            0 S L15 AND SILICONE
L20            0 S L15 AND CUTANEOUS?
L21            0 S L15 AND ACCELERAT?
L22            1 S L9
L23            4 S L12
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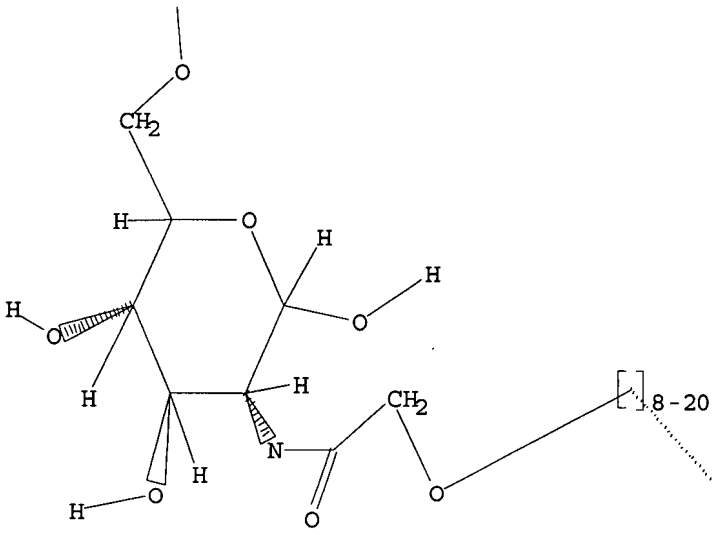
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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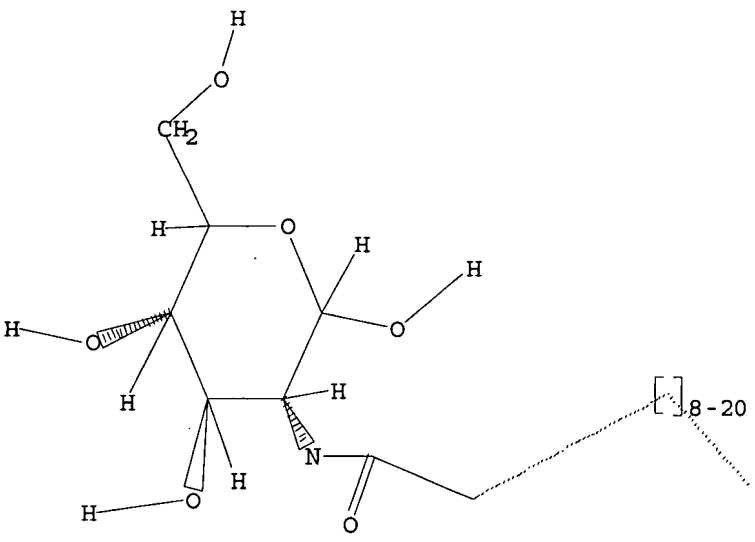
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

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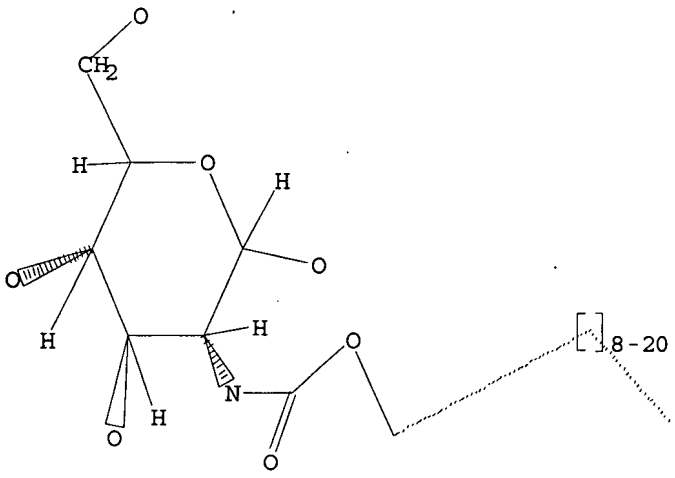
L7 STR



Structure attributes must be viewed using STN Express query preparation.

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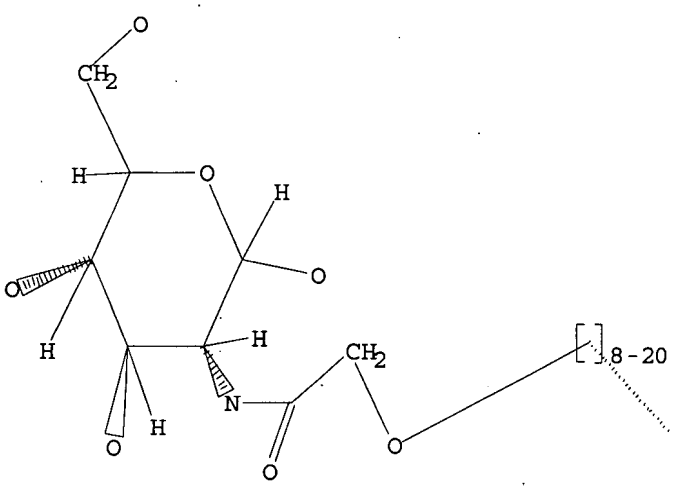
L10 STR



Structure attributes must be viewed using STN Express query preparation.

L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:341537 CAPLUS
DOCUMENT NUMBER: 129:32158
TITLE: Novel pseudoceramides and dermatologic external preparations containing them
INVENTOR(S): Park, Byeong Deog; Baik, In Sob; Lee, Jong Gi; Kim, Yoon; Lee, Myung Jin
PATENT ASSIGNEE(S): Ae Kyung Industrial Co., Ltd., S. Korea; Park, Byeong Deog; Baik, In Sob; Lee, Jong Gi; Kim, Yoon; Lee, Myung Jin
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9821176	A1	19980522	WO 1997-KR220	19971110
W: CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2001509138	T	20010710	JP 1998-522409	19971110
KR 2000052640	A	20000825	KR 1999-703408	19990419
US 6221371	B1	20010424	US 1999-308031	19990510
PRIORITY APPLN. INFO.:			KR 1996-53207 A	19961111
			WO 1997-KR220 W	19971110

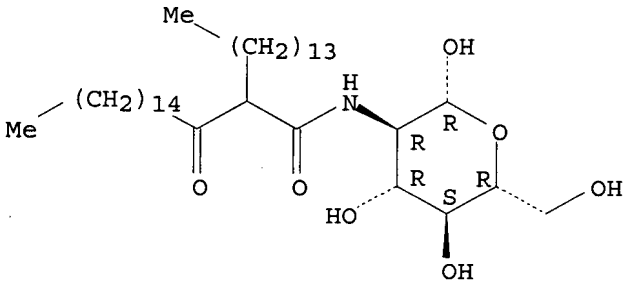
OTHER SOURCE(S): MARPAT 129:32158

AB Pseudoceramide derivs. R1COCHR2CONR3R4 or R1CH(OH)CHR2CONR3R4 (R1, R2 = linear or branched C6-22 alkyl or alkenyl group; R3, R4 = H, Me, Et, Pr, linear or branched C2-6 alkyl group having ≥1 OH group, or monosaccharide) are prepared When the pseudoceramide derivs. are applied in a dermatol. external preparation the moisture-retaining property and resilience of skin and hair becomes excellent so that the derivs. are useful in protection of skin-aging. Besides, the derivs. are useful for inducing the formation of lipid layer on damaged skin and for preventing the inhibition of lipid synthesis.

IT 208044-60-4P
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pseudoceramides and dermatol. external prepns.)

RN 208044-60-4 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1,3-dioxo-2-tetradecyloctadecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

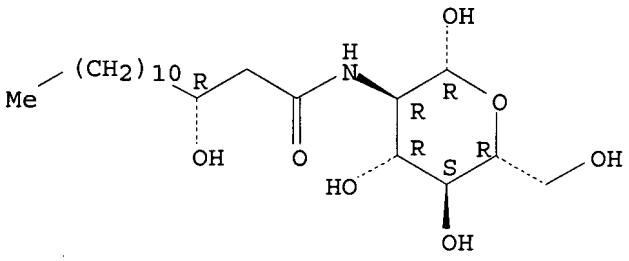
L15 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1985:452604 CAPLUS
DOCUMENT NUMBER: 103:52604
TITLE: Chemical synthesis and immunological activities of glycolipids structurally related to lipid A
AUTHOR(S): Charon, Daniel; Chaby, Richard; Malinvaud, Agnes; Mondange, Michelle; Szabo, Ladislas
CORPORATE SOURCE: Inst. Biochim., Univ. Paris Sud, Orsay, 91405, Fr.
SOURCE: Biochemistry (1985), 24(11), 2736-42
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Complete chemical syntheses of a number of monosaccharides derived from 2-deoxy-2-[(3R)-3-hydroxytetradecanamido]-D-glucopyranose and structurally related to the hydrophobic moiety (lipid A) of several bacterial endotoxins are described. Selected humoral (complement activation) and cellular (mitogenicity and induction of interleukin 1 production) in vitro activities of a lipid A preparation obtained from the Bordetella pertussis endotoxin were compared with those of 10 of these monosaccharides and with those of previously synthesized, analogous disaccharides. Each of these in vitro activities of the lipid A preparation can be efficiently induced by at least one of the monosaccharide derivs.

IT 96151-64-3DP, albumin conjugates 96151-64-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and immunol. activity of, lipid A in relation to)

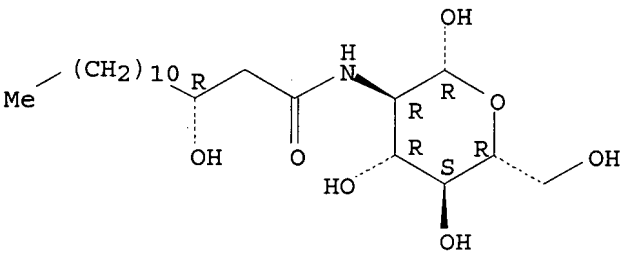
RN 96151-64-3 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(3-hydroxy-1-oxotetradecyl)amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 96151-64-3 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(3-hydroxy-1-oxotetradecyl)amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



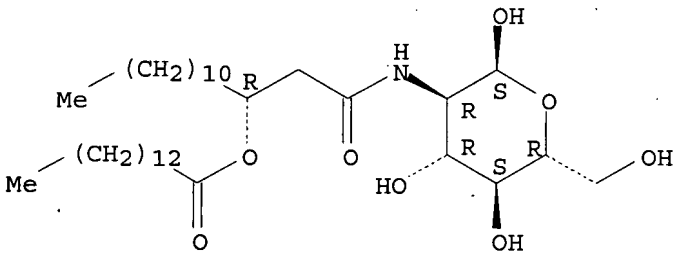
L15 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:585656 CAPLUS
DOCUMENT NUMBER: 101:185656

TITLE: Mitogenic activities of synthetic lipid A analogs and suppression of mitogenicity of lipid A
AUTHOR(S): Tanamoto, Kenichi; Galanos, Chris; Luederitz, Otto; Kusumoto, Shoichi; Shiba, Tetsuo
CORPORATE SOURCE: Max-Planck-Inst. Immunbiol., Freiburg, D-7800, Fed. Rep. Ger.
SOURCE: Infection and Immunity (1984), 44(2), 427-33
CODEN: INFIBR; ISSN: 0019-9567
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of synthetic lipid A analogs on murine spleen cells was studied. The prepns. represented D-glucosamine and D-glucosaminyl-β-1,6-D-glucosamine disaccharide derivs. substituted in different combinations by ester- and amide-bound fatty acids and by phosphate groups. Significant mitogenic activity was demonstrated with a number of synthetic disaccharide prepns.; however, their potency was lower than that of lipid A. The synthetic prepns. were not mitogenic for spleen cells from C3H/HeJ mice. The mitogenicity of the synthetic prepns. was abolished after binding with polymyxin B. A phoshate group at position 1 of the reducing glucosamine and amide-bound acyloxyacyl residues are important factors for the expression of mitogenicity. Some of the synthetic prepns. containing the diglucosamine backbone and expressing relatively low mitogenicity suppressed B-cell mitogenicity of lipid A. Although these prepns. were lytic for erythrocytes, they did not affect the viability of the splenic lymphocytes. Suppression was seen when the synthetic prepns. were added simultaneously with or after the lipid A mitogen, but optimal suppression was expressed when the prepns. were added to the system 3 h before lipid A. Washing of the cells before the addition of lipid A did not affect the results. The suppression was not due to the induction of suppressor cells by the synthetic prepns. The disaccharide prepns. did not inhibit T-cell mitogenicity of Con A. The monosaccharide prepns. suppressed mitogenicity of both lipid A and Con A, probably because of their direct toxicity for lymphocytes.

IT 91732-64-8
RL: BIOL (Biological study)
(mitogenicity of, lipid A in relation to)
RN 91732-64-8 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:505463 CAPLUS
DOCUMENT NUMBER: 101:105463
TITLE: Biological activities of synthetic lipid A analogs: pyrogenicity, lethal toxicity, anticomplement activity, and induction of gelation of Limulus amoebocyte lysate
AUTHOR(S): Tanamoto, Kenichi; Zaehringer, Ulrich; McKenzie, Gerry R.; Galanos, Chris; Rietschel, Ernst T.; Luederitz, Otto; Kusumoto, Shoichi; Shiba, Tetsuo

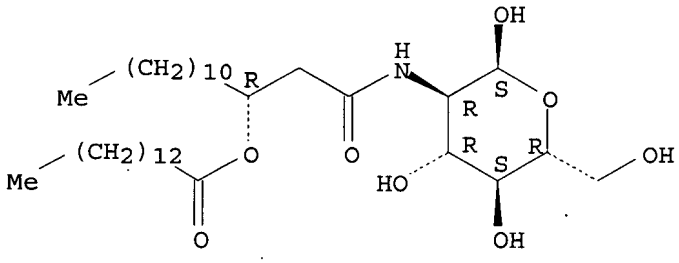
CORPORATE SOURCE: Max-Planck-Inst. Immunbiol., Freiburg, D-7800, Fed. Rep. Ger.
SOURCE: Infection and Immunity (1984), 44(2), 421-6
CODEN: INFIBR; ISSN: 0019-9567
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Chemical synthesized lipid A analogs were investigated for several endotoxic activities, including pyrogenicity, lethal toxicity, anticomplement activity, and the capacity to gelate Limulus amebocyte lysate in comparison to natural lipid A. The synthetic prepns. contained D-glucosamine or D-glucosamine-β-1,6-D-glucosamine disaccharide substituted by ester- and amide-bound hydroxylated or nonhydroxylated fatty acids and by phosphate groups in different combinations. Some prepns. which were insol. in water were succinylated and thus rendered more soluble Strong biphasic pyrogenic responses with a maximal increase in body temperature of 1-2° were obtained with 50 μg/kg doses of 3 disaccharide prepns. of 15 tested. With 2 prepns. (50 μg/kg) moderate pyrogenicity with monophasic fever curves and a maximal temperature increase of .apprx.0.6° was obtained. Lethal toxicity tests were carried out in galactosamine-sensitized mice. Of 15 synthetic prepns., 4 exhibited lethal toxicity under these conditions. The EDs of the lipid A analogs in both in vivo tests were, however, several hundred times higher than those of bacterial lipid A. For the activities in vivo, hydroxyacyl residues seemed to be important. Anticomplement activity was demonstrable in 7 prepns., 1 of which expressed an activity comparable to that of lipid A. Prepns. containing nonhydroxylated fatty acids seemed to be most active in this test. None of the synthetic prepns. was found to exhibit gelation activity for Limulus amebocyte lysate when tested in doses up to 0.4 μg, whereas bacterial free lipid A was active in doses of .apprx.2 pg. None of the monosaccharide derivs. exhibited any of these activities.

IT 91732-64-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(endotoxic activity of, lipid A in relation to)

RN 91732-64-8 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:451078 CAPLUS
DOCUMENT NUMBER: 101:51078
TITLE: Laser desorption mass spectrometry of synthetic lipid A-like compounds
AUTHOR(S): Seydel, Ulrich; Lindner, Buko; Zaehringer, Ulrich; Rietschel, Ernst T.; Kusumoto, Shoichi; Shiba, Tetsuo
CORPORATE SOURCE: Forschungsinst. Borstel, Borstel, D-2061, Fed. Rep. Ger.
SOURCE: Biomedical Mass Spectrometry (1984), 11(3), 132-41
CODEN: BMSYAL; ISSN: 0306-042X
DOCUMENT TYPE: Journal

LANGUAGE: English

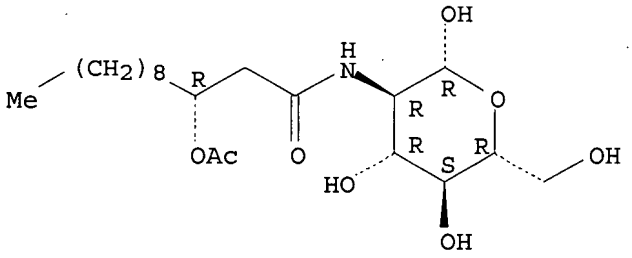
AB The applicability and the present limitations of the laser microprobe mass analyzer LAMMA-500 as an instrument for the structural anal. of higher-mol.-weight, nonvolatile, bioorg. compds. (≤2000 amu) were investigated. For this purpose, mass spectra of various synthetic and natural compds. representing cell wall components of gram-neg. bacteria, e.g., phospholipids and lipid A-like mols., were studied. In several cases, these spectra exhibited relatively simple and interpretable patterns with a prominent quasi-mol. ion originating from alkali attachment. For 1 group of the compds. studied (synthetic lipid A-like mols. containing a phosphate moiety), the spectra were rather complicated and lacked pronounced quasi-mol. peaks. Possible reasons for this observation are discussed.

IT 90996-43-3
RL: PRP (Properties)
(mass spectrum of)

RN 90996-43-3 CAPLUS

CN β-D-Glucopyranose, 2-[[3-(acetyloxy)-1-oxododecyl]amino]-2-deoxy-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1982:144928 CAPLUS

DOCUMENT NUMBER: 96:144928

TITLE: Monolayers from synthetic glycolipids

AUTHOR(S): Emmerling, W. N.

CORPORATE SOURCE: Inst. Makromol. Chem., Univ. Freiburg, Freiburg/Br., 7800, Fed. Rep. Ger.

SOURCE: Polymer Bulletin (Berlin, Germany) (1982), 6(5-6), 305-8
CODEN: POBUDR; ISSN: 0170-0839

DOCUMENT TYPE: Journal

LANGUAGE: English

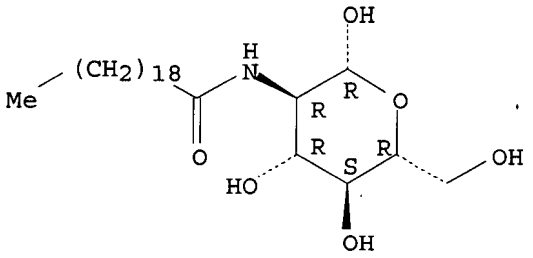
AB Synthetic glycolipids were prepared by (a) coupling of aliphatic amines RNH2 [R = C12H25, C18H37, Br(CH2)12, Br(CH2)20, F3C(CF2)11CH2CH2] with lactone derivs. (gluconolactone or maltobionic acid lactone), or (b) Me(CH2)18CO2H with saccharide amino derivs. (e.g., 2-deoxy-2-aminoglycose) via an amide linkage. The influence of the glycolipid structure on monolayer properties was studied. Stable films were obtained with most of the products due to strong interactions by H bonds in the subphase. Polymeric films may be produced by polycondensation in the subphase using crosslinking agents for the carbohydrate head group.

IT 81313-53-3
RL: USES (Uses)
(film, monolayer properties of)

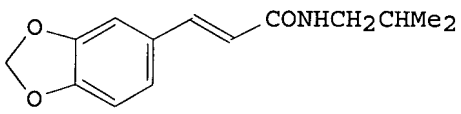
RN 81313-53-3 CAPLUS

CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxoeicosyl)amino]- (9CI) (CA INDEX NAME)

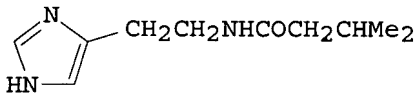
Absolute stereochemistry.



L15 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:604909 CAPLUS
Correction of: 1980:426592
DOCUMENT NUMBER: 93:204909
Correction of: 93:26592
TITLE: Studies on a new synthesis of the acyclic amide and macrocyclic lactam alkaloids
AUTHOR(S): Nagao, Y.; Seno, K.; Miyasaka, T.; Kawabata, K.; Takao, S.; Fujita, E.
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, Japan
SOURCE: Koen Yoshishu - Tennen Yuki Kagobutsu Toronkai, 22nd (1979), 554-61. Kyushu Univ., Fac. Sci., Dep. Chem.: Fukuoka, Japan.
CODEN: 42MAAQ
DOCUMENT TYPE: Conference
LANGUAGE: Japanese
GI



I



II

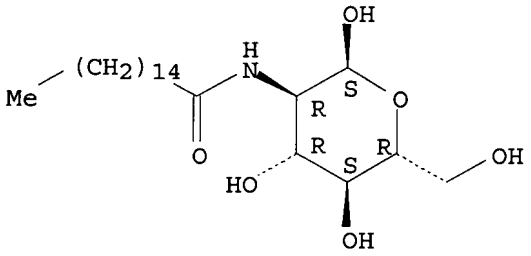
AB Aminolysis of 3-acylthiazolidine-2-thiones gave high yields of amides, e.g. Me(CH2)14CONHBu, and aminolysis of 3-hexadecanoylthiazolidine-2-thione with amino alcs. gave hydroxy amides in satisfactory yields. Naturally occurring amide alkaloids, fagaramide (I), dolichotheline (II), and maytenine, HN[(CH2)3NHCOCH=CHPh]2, were prepared by the application of this aminolysis reaction. Macrocyclic lactams was also prepared

IT 74058-79-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

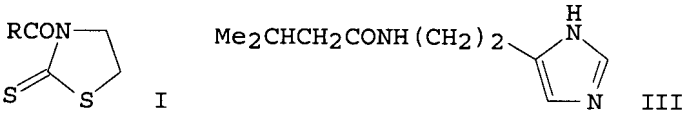
RN 74058-79-0 CAPLUS

CN α-D-Glucopyranose, 2-deoxy-2-[(1-oxohexadecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

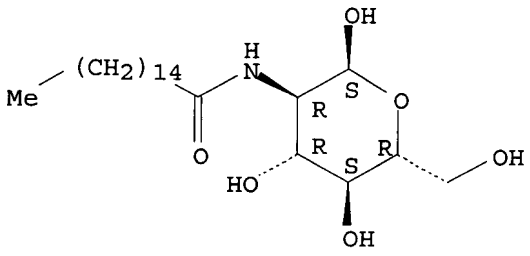


L15 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:470972 CAPLUS
DOCUMENT NUMBER: 93:70972
TITLE: Monitored aminolysis of 3-acylthiazolidine-2-thione: a new convenient synthesis of amide
AUTHOR(S): Nagao, Yoshimitsu; Seno, Kaoru; Kawabata, Kohji; Miyasaka, Tadayo; Takao, Sachiko; Fujita, Eiichi
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611, Japan
SOURCE: Tetrahedron Letters (1980), 21(9), 841-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

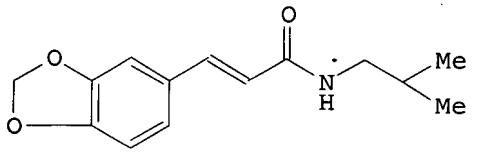


AB 3-Acylthiazolidine-2-thiones reacted with amines in CH2Cl2 giving high yields of the corresponding amides. E.g., the thione I [R = Me(CH2)14] (II) reacted with BuNH2 (1 min), giving 96% Me(CH2)14CONHBu. Amino alcs. and aminophenols were similarly selectively converted into amido alcs. and amidophenols, resp. E.g., HOCH2CH2NH2 and 4-HOC6H4NH2 reacted with II giving 91% HOCH2CH2NHCO(CH2)14Me and 63% 4-HOC6H4NHCO(CH2)14Me, resp. Four amido alkaloids were prepared using this procedure. E.g., Me2CHCH2COCl reacted with thiazolidine-2-thione giving 89% I (R = Me2CHCH2) which reacted with histamine giving 73% dolichotheline (III).
IT 74058-79-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74058-79-0 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[(1-oxohexadecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:426592 CAPLUS
DOCUMENT NUMBER: 93:26592
TITLE: Studies on a new synthesis of the acyclic amide and macrocyclic lactam alkaloids
AUTHOR(S): Nagao, Y.; Seno, K.; Miyasaka, T.; Kawabata, K.; Takao, S.; Fujita, E.
CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, Japan
SOURCE: Koen Yoshishu - Tennen Yuki Kagobutsu Toronkai, 22nd (1979), 554-61. Kyushu Univ., Fac. Sci., Dep. Chem.: Fukuoka, Japan.
CODEN: 42MAAQ
DOCUMENT TYPE: Conference
LANGUAGE: Japanese
GI

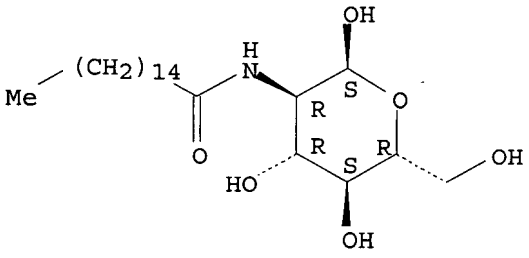


I

AB An efficiently monitored aminolysis of 3-acylthiazolidine-2-thione gave a very high yield of amines. The similar aminolysis of 3-hexadecanoylthiazolidine-2-thione with aminoalcs. resulted in the formation of hydroxyamides in satisfactory yields. Thus, naturally occurring amide alkaloids, fagaramide (I), dolichotheline, and maytenine, were synthesized in good yields by the application of the foregoing aminolysis. Synthesis of macrocyclic lactams was also successfully carried out.

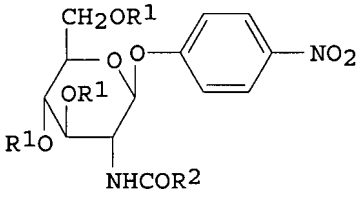
IT 74058-79-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74058-79-0 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[(1-oxohexadecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:406003 CAPLUS
DOCUMENT NUMBER: 85:6003
TITLE: Synthesis of some p-nitrophenyl 2-acylamino-2-deoxy-D-glucosides and their hydrolysis with the β-D-hexosaminidase from Hohenbuehelia serotina
AUTHOR(S): Vafina, M. G.; Molodtsov, N. V.
CORPORATE SOURCE: Pac. Inst. Bio-Org. Chem., Vladivostok, USSR
SOURCE: Carbohydrate Research (1976), 47(1), 188-94

CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:6003
GI



I

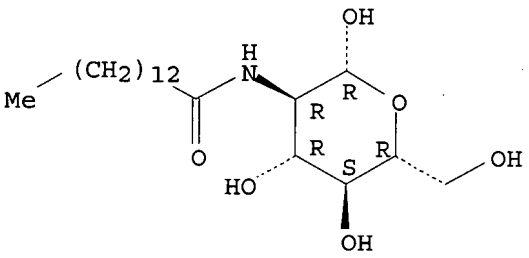
AB Treatment of 2-amino-2-deoxy-D-glucose with fatty acids, their chlorides, or anhydrides followed by acetylation and treatment with NaOC6H4NO2-4 in DMF gave I (R1 = Ac, R2 = (CH2)nH, n = 0-13). Deacetylation gave I (R1 = H, R2 = (CH2)nH, n = 0-13) which were hydrolyzed with β-D-hexosaminidase.

IT 59343-85-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)

RN 59343-85-0 CAPLUS

CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxotetradecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:461382 CAPLUS
DOCUMENT NUMBER: 75:61382
TITLE: Immunological properties of synthetic sugar-polypeptide conjugates. Effect of N-lauroylglucosamine residues on immunogenicity
AUTHOR(S): Ruede, E.; Meyer-Delius, Margot; Gundelach, Maria L.
CORPORATE SOURCE: Max-Planck-Inst. Immunbiol., Freiburg/Br., Fed. Rep. Ger.
SOURCE: European Journal of Immunology (1971), 1(2), 113-23
CODEN: EJIMAF; ISSN: 0014-2980
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several mono- and disaccharides were tested for their capacity to enhance the immunogenicity of a weakly immunogenic synthetic polypeptide by attaching them to the side chains of multichain poly-DL-alanine as O-glycosides of serine. Among the sugar conjugates tested, the glucose, N-acetylglucosamine, and lactose conjugates were essentially nonimmunogenic while the rhamnose, galactose, and cellobiose conjugates were only slightly better immunogens than the unsubstituted polypeptide.

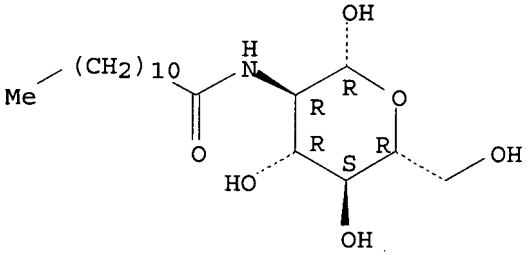
The antibodies elicited were directed almost entirely against the serine glycoside residues. The effect of lipids on the immunogenicity of sugar-polypeptide conjugates was also studied by incorporation of N-lauroylglucosaminyl-serine residues in addition to the usual sugars. In all cases this led to an increase in immunogenicity, perhaps due in part to the high degree of aggregation of these polymers. In most of the polymers the N-lauroylglucosaminyl-serine residues also functioned as determinant groups and the fatty acid residue played an important role in interaction with antibody.

IT 33600-58-7
RL: BIOL (Biological study)
(hapten, as antigenic determinant)

RN 33600-58-7 CAPLUS

CN Glucopyranose, 2-deoxy-2-lauramido-, β-D- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1956:77523 CAPLUS

DOCUMENT NUMBER: 50:77523

ORIGINAL REFERENCE NO.: 50:14541a-i,14542a-i,14543a-i,14544a-e

TITLE: Synthetic emulsifying agents

AUTHOR(S): Fieser, Mary; Fieser, Louis F.; Toromanoff, Edmond; Hirata, Yoshimasa; Heymann, Hans; Tefft, Melvin; Bhattacharya, Sivaprasad

CORPORATE SOURCE: Harvard Univ.

SOURCE: Journal of the American Chemical Society (1956), 78, 2825-32
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB C18H37OH (10.8 g.) in 180 cc. CHCl3 added slowly with vigorous stirring and cooling to 6 cc. PhP(O)Cl2 in 16 cc. CHCl3 and 3.4 cc. pyridine, the mixture warmed 10 min. at 35°, treated with 5.6 g. dry powdered HO(CH2)2NMe3Cl, stirred 48 hrs. at room temperature, and evaporated, the residue extracted with three 50-cc. portions Et2O, the insol. residue dissolved in 50 cc. H2O, the solution saturated with NaCl and extracted with CHCl3, and the extract evaporated yielded 7 g. C18H37OP(O)(OPh)OCH2CH2NMe3Cl (I), m. 82-6° (from Me2CO). I (3.0 g.) hydrogenated in EtOH over PtO2 yielded 1.8 g. C18H37OP(O)(OH)OCH2CH2NMe3Cl (Ia) m. 71-2° (from Me2CO). Ia in EtOH treated with Amberlite IRA-400, the solvent partially removed, the residue diluted with Me2CO, and the crude precipitate chromatographed and eluted with 4:1 CHCl3-EtOH gave the corresponding hydroxide, m. 220-30°; it is sparingly soluble in H2O and Nujol at room temperature and shows no emulsifying properties. Dihydrophytyl and cholestanyl phosphorylcholine were prepared in essentially the same manner but could not be obtained pure; the crude dihydrophytyl derivative (semisolid) showed some emulsifying action. L-Arabinose (75 g.) in H2O treated at room temperature 12 hrs. with 120 g. Br, the excess Br removed in vacuo at 40-50°, the mixture treated with

120 g. PbO, the white precipitate filtered off after several hrs., the filtrate treated dropwise with H_2SO_4 and filtered, concentrated in vacuo at 50°, and the residue diluted with 75 cc. MeOH and allowed to stand a few hrs. at 5° deposited 77% arabonolactone (II), m. 148-50° (from MeOH), αD^{30} -6.5°. II (2 g.) in MeOH treated with 2.2 g. $C_{12}H_{25}NH_2$ and kept at room temperature deposited 87.5% N-laurylarabonamide, m. 150-1° (from EtOH or dioxane). Similarly were prepared the following N-alkylarabonamides (alkyl group and m.p. given): $C_{10}H_{21}$, 150-1° (from EtOH); $C_{14}H_{29}$, 150-1° (from EtOH); $C_{16}H_{33}$, 150-1° (from dioxane); $C_{18}H_{37}$, 149-50° (from dioxane). Gluconolactone condensed with $C_{18}H_{37}NH_2$ (IIa) at 140° or in refluxing EtOH during 1 hr. gave N-stearylgluconamide, m. 149.4-54.8° (from EtOH). Similarly were prepared the following N-alkylgluconamides (III) (alkyl group and m.p. given): $C_{12}H_{25}$, 153.2-5.6°; $C_{16}H_{32}$, 150.4-4.6°. Glucoheptonolactone (2.08 g.), m. 148-52°, and 2.69 g. IIa gave similarly 55% N-stearylglucoheptonamide, m. 149-52° (cloudy) (from EtOH); it decomposed at about 180°. The C14-, C16-, and C18-III gave a solubility of about 6 g./l. boiling H_2O; when used with cholesterol or the mono-stearyl ether of $(CH_2OH)_2$ emulsions with an average particle size of 5-10 μ can be obtained in a Waring Blendor; these emulsions are stable only for a few hrs. 1,2-Isopropylideneglucuronolactone (IV) was prepared in 81% yield by the method of Owen, et al. (C.A. 35, 6240.2), except that the volume of Me_2CO was reduced to 500 cc. for 20 g. IV and Na_2CO_3 was used instead of $BaCO_3$. IV (6.6 g.) in 50 cc. dioxane and 15 cc. cold concentrated NH_4OH kept 4-5 hrs. in the cold room, and the solution evaporated in vacuo below 45° gave almost 100% 1,2-isopropylideneglucuronamide (V), needles, m. 163-4° (from absolute EtOH), αD^{18} -13.5° (c 1, H_2O). IV (5.8 g.) in 50 cc. dry tetrahydrofuran treated with 6.8 g. IIa in small portions with stirring, kept overnight in the cold room, and then a few hrs. at room temperature, the solvent removed in vacuo below 40° to incipient crystallization, and the residue diluted with petr. ether gave 8.0 g. 1,2-isopropylidene-N-stearylglucuronamide (VI), m. 92-3°; 2nd crop, 2.3 g., m. 86-90°. Similarly were prepared the following 1,2-isopropylidene-N-alkylglucuronamides in 70-90% yield (alkyl group, m.p., and αD in MeOH given): $C_{10}H_{21}$, 70-5° (from petr. ether), -14° (c 1.162); $C_{12}H_{25}$, 87-8° (from MeOH), -13° (c 1.046); $C_{14}H_{29}$, 88-90° (from MeOH), -12.5° (c 1.09); $C_{16}H_{33}$, 90-2° (from EtOH), -13.5° (c 1.064). ω-Cyclohexyldecanoic acid (10 g.) refluxed 2 hrs. with 15 cc. $SOCl_2$ and evaporated in vacuo, and the cooled residue poured slowly into 100 cc. ice-cold concentrated NH_4OH yielded 9 g. ω-cyclohexyldecanamide (VII), m. 89-93° (from aqueous MeOH). VII (7.6 g.) reduced in the usual manner with $LiAlH_4$ in refluxing Et_2O and the Et_2O solution treated with HCl gave 6.3 g. ω-cyclohexyldecylamine HCl salt, m. 151-3° (from MeOH); free base, m. above 50°. The free amine in Et_2O (liberated with aqueous $NaHCO_3$ from the HCl salt) treated with IV gave 1,2-isopropylidene-N-(ω-cyclohexyldecyl)glucuronamide, m. 88-90°. V (2.3 g.) in 20 cc. H_2O and 0.5 cc. concentrated HCl heated 1-3 min. at 80°, the H_2O removed in vacuo, and the residue crystallized from absolute MeOH gave 1.8 g. glucuronamide (VIII).H_2O, m. 168-9° (decomposition), αD^{22} 70° → 31.9° (44 hrs., c 1.77, H_2O); anhydrous VIII, m. 173-4°. γ-Lactone of β-methylglucuronoside (4.2 g.) in 20 cc. cold dioxane treated overnight with 10 cc. ice cold NH_4OH (d. 0.9), the solvent removed in vacuo below 40°, and the residue hydrolyzed with HCl gave 2.1 g. VIII.H_2O. VI (5 g.) in 100-350 cc. H_2O and 7 cc. concentrated HCl tested with stirring 30-45 min. on the steam bath and the mixture cooled gave the corresponding N-alkylglucuronamides (alkyl group, m.p., and αD in MeOH given): $C_{10}H_{21}$, 145-8° (decomposition) (from aqueous MeOH), 24° (c 1.11); $C_{12}H_{25}$, 160-1° (from aqueous dioxane), -4° → 22° (24 hrs., c 1.18); $C_{14}H_{29}$, 156-7° (from aqueous dioxane), 11° → 24° (24 hrs., c 1.05); $C_{16}H_{33}$ (IX), 155-7° (from aqueous dioxane), 24.7° →

26° (24 hrs., c 1.03); C18H37 (X), 153-4° (from aqueous dioxane), 23° (10 min., c 1.046); ω-cyclohexyldecyl (XI), 128-30° (from MeOH), 21° → 25° (24 hrs., c 1.15). ω-Cyclohexylbutyramide, m. 103-6°, reduced to the amine (HCl salt, m. 165-7°), condensed with V, and the product hydrolyzed yielded 80% ω-cyclohexylbutylglucuronamide, m. 160-3° (from aqueous MeOH), αD 35.8° → 23.5° (24 hrs., c 1.54, MeOH). IX, X, and XI gave fairly stable oil-in-water emulsions when used with a co-emulsifier. IIa (2.5 g.) in 15 cc. cold tetrahydrofuran added to 2 g. β-methylglucuronoside-γ-lactone in cold tetrahydrofuran, the mixture kept overnight in the cold room and then 1-2 hrs. at room temperature, and the solvent removed in vacuo yielded 77% N-stearylamide (XII) of β-methylglucuronoside (XIII), m. 75-8° (from Et2O), αD21 -60.4° (c 1.03, MeOH). A similar run carried out at an initial temperature of 40-50° for 0.5 hr. and then at 25° for 2-3 hrs. yielded 87% higher melting form of XII, m. 93-5° (from MeOH-C6H6), αD25 -60.7° (c 1.0, MeOH). Similarly were prepared the following N-alkylamides of XIII (alkyl group, m.p., and αD in MeOH of form A and B given): C12H25, 68-70°, -58.4° (c 1.05), 88-90°, -58.7° (c 1.43); C14H29, 70-3°, -60.8° (c 1.11), 88-90°, -61° (c 1.04); C16H33, 75-8°, -60.6° (c 1.3), 92-3°, -60.5° (c 1.3). The glucuronosides were hydrolyzed with 1 cc. concentrated HCl in 100 cc. H2O to the corresponding glucuronamides in nearly 100% yield. The appropriate glucuronamide (5 g.) in 250-500 cc. hot H2O treated at 50-60° with 4 cc. Br at 40-50°, the solution kept in the cold room overnight, the excess Br removed with saturated aqueous Na2S2O3, and the product air-dried and recrystd. from tetrahydrofuran gave about 80% of the corresponding N-alkylglucosaccharonamide (XIV) (alkyl group, m.p., and αD in tetrahydrofuran given): C12H25, 134-7°, -21.5° (c 1.13); C14H29, 125-7°, -22° (c 1.06); C16H33, 135-8° with previous sintering, -21° (c 1.14); C18H37, 137-9°, -22° (c 1.12). The XIV gave less stable emulsions than the corresponding glucuronamides; they are slightly more H2O-soluble C11H23COCl (2.2 g.) in 20 cc. tetrahydrofuran added dropwise with stirring to 2.15 g. glucosamine.HCl salt and 2 g. NaHCO3 in 20 cc. H2O with agitation, the mixture agitated 0.5 hr. and diluted with 100 cc. H2O, and the precipitate washed with H2O and recrystd. from dioxane-EtOH gave 3.2 g. N-lauroylglucosamine, m. 190-3°. Similarly were prepared the following N-acylglucosamines (XV) (acyl group and m.p. with decomposition given): C13H27CO, 193-5° (from dioxane-EtOH); C15H31CO, 190-3° (from dioxane-EtOH); C17H35CO, 190-1° (from dioxane-EtOH). C17H35CO2H (XVI) (11.4 g.) and 6 cc. Et3N in dry tetrahydrofuran treated with stirring and cooling at -5° with 4 cc. ClCO2Et and then after 5 min. without further cooling with the Na salt of 3.6 g. β-alanine in 30 cc. cold H2O, the mixture stirred 0.5 hr., acidified to pH 3-4, and filtered, and the residue washed with warm H2O, dried, extracted with petr. ether, and recrystd. from 4:1 dioxane-H2O or tetrahydrofuran yielded 11.2 g. stearoyl-β-alanine (XVII), m. 122-4°, insol. in H2O at 25°, somewhat soluble at 100°. In the same manner was prepared oleoyl-β-alanine (XVIII), m. 75-6° (from aqueous dioxane). XVIII (1 g.), 1.2 g. AgOAc, and 13 cc. glacial AcOH containing 0.1 cc. H2O treated during 40 min. with 0.72 g. iodine, the mixture heated 3 hrs. on the steam bath, cooled, filtered, and evaporated, the residue in MeOH refluxed 25 min. with aqueous KOH and filtered, and the filtrate acidified gave 0.6 g. 9,10-dihydroxystearoyl-β-alanine, m. 148-50° (from EtOH). XVII was converted in the usual manner in 71% yield to stearoyl-β-alanyl-β-alanine, m. 153-6° (from aqueous dioxane). Similarly were prepared: stearoyl-β-alanylglycine, 75%, m. 172-4° (from dioxane-H2O); stearoyl-β-alanyltaurine, 78%, m. about 200° (decomposition) (it contains solvent of crystallization which is not removed by drying at 150°). XVI (3 g.), 1.07 g. Et3N, and 1.44 g. ClCO2CH2CHMe2 in CHCl3-EtOAc treated with 1.62 g. α-alanine Et ester (XVIIIa) HCl

salt and 1.07 g. Et3N gave 2.87 g. stearoyl-α-alanine Et ester (XIX), m. 62-5° (from ligroine). XIX (1 g.) in 10 cc. dioxane hydrolyzed with 3 cc. concentrated HCl in 1.5 cc. H2O on the steam bath during 1 hr. yielded 0.63 g. DL-stearoyl-α-alanine (XX), m. 115-17° (from ligroine-dioxane). XX and XVIIIa were converted by the mixed anhydride method to stearoyl-α-alanyl-α-alanine Et ester, m. 82-3°, which was hydrolyzed to the free acid, m. 132-3° (from petr. ether-dioxane). Similarly were prepared the following compds. (% yield and m.p. given): stearoylglycine (XXI), 75-80, 125-7° (from EtOAc-tetrahydrofuran); stearoylglycyl-β-alanine, 70-5, 169-70° (from dioxane); stearoylglycylglycine, 75-80, 170-2° (from dioxane); stearoylglycyltaurine, 80-90, -(practically insol. in various organic solvents; it crystallized from H2O with H2O of crystallization which is not lost by drying at 150°); stearoyltaurine, 73, m. about 240° (decomposition); stearoyl-DL-asparagine (XXII), 70, 145-8° (from dioxane); stearoylglycylasparagine (XXIII).H2O, 70-5°, 180-5° (from aqueous dioxane). XXII (0.4 g.) in 10 cc. dioxane treated with 0.08 g. NaNO2 in 30 cc. H2O, warmed 4-6 hrs. on the steam bath with 0.4 cc. concentrated HCl, and cooled to room temperature deposited 0.37 g. stearoyl-DL-aspartic acid (XXIV), m. 111-13° (from aqueous dioxane or EtOAc). XXIV heated 15 min. at 70-80° in Ac2O and cooled gave 100% stearoyl-DL-aspartic anhydride, m. 124-5° (from ligroine containing some tetrahydrofuran). Stearoyl-L-glutamic acid, m. 127-8° (from tetrahydrofuran), αD22 8.5° (c 1.62, dioxane), was prepared in 55% yield by the mixed anhydride method from L-glutamic acid and then converted in the usual manner to the anhydride, m. 107-9° (from ligroine-tetrahydrofuran). XXIII hydrolyzed with acid in the presence of NaNO2 yielded 80-90% stearoyl-DL-aspartic acid, m. 165-70°; also prepared in 40-60% yield directly from XXI; the acid was converted in the usual manner to the anhydride, m. 175-80°. C18H32CHBrCO2H (10 g.) heated 24 hrs. with excess 27% NH4OH in a pressure bottle and the product washed with H2O and boiling MeOH and ligroine gave 8.5 g. C16H33CH(NH2)CO2H (XXV), m. 223-4° (decomposition). XXV heated with phthalic anhydride 0.5 hr. at 145-60° gave the phthalimido derivative (XXVI) of XXV, m. 81° (from ligroine). XXVI (2 g.) refluxed 3 hrs. with 10 cc. SOCl2, the excess SOCl2 removed with suction, the residual oil washed with dry PhMe, dried at 1 mm., dissolved in 20 cc. dry CHCl3, and treated with 0.71 g. Et ester of α-alanine HCl salt in 10 cc. dry CHCl3, the mixture cooled to -20°, treated with stirring during 40 min. with 1.1 g. Et3N in dry CHCl3, warmed to room temperature, and evaporated in vacuo, and the residue dissolved in ligroine, washed with H2O, evaporated, and diluted with petr. ether yielded 0.9 g. Et ester (XXVII) of α-phthalimidostearoyl-α-alanine (XXVIII), crystals, m. 63-4°; XXVIII, m. 116° (from ligroine). XXVIII (0.45 g.) in 7 cc. 95% EtOH refluxed 45 min. with 1.5 cc. N2H4 and a few drops H2O, cooled, and diluted with H2O gave 0.28 g. α-aminostearoyl-α-alanine, m. 218-20°. N-Carbobenzyloxy-DL-alanine (4.46 g.), m. 120-2° in 50 cc. tetrahydrofuran containing 3 cc. Et3N treated with stirring at -5° with 5.4 g. IIa in 50 cc. tetrahydrofuran, the mixture stirred 0.5 hr. without cooling and acidified, the solvent partially removed in vacuo, the residue diluted with cold H2O, and the precipitate washed with cold dilute NH4OH and recrystd. from MeOH yielded 8 g. N-carbobenzyloxy-DL-alanylstearylamine (XXIX), m. 106-9°. XXIX (4.7 g.) in 100 cc. absolute MeOH hydrogenated overnight over 0.25 g. 10% Pd-C, filtered, and evaporated, and the residue heated a few hrs. at 80-90° gave DL-alanylstearylamine (XXX), m. 76-8° (from MeOH). Similarly were prepared the following dipeptides (m.p. and m.p. of the N-carbobenzyloxy derivative given): L-isomer of XXX, 70-3° (from Et2O), 103-4° (from MeOH); L-alanylcetylamine.0.5 H2O, 58-60° (from Et2O), m. 90-30 (from MeOH); L-alanyl-ω-cyclohexyldecylamine, 56-8° (from MeOH), 115-16° (from

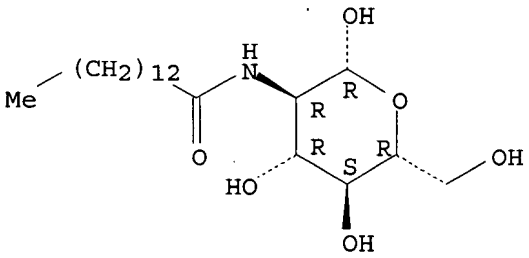
MeOH); L-leucylstearylamine, 66-8° (from MeOH), (hemihydrate) 96-8° (from MeOH); L-leucylcetylamine, 58-60° (from MeOH), 95-7° (from MeOH); L-prolylstearylamine, 70-2° (from MeOH), 88-90° (from MeOH); glycylstearylamine hemihydrate, 96-8° (from MeOH), 116-18° (from tetrahydrofuran); glycylcetylamine, 84-6° (from MeOH), 110-11° (from MeOH); β-alanylstearylamine hemihydrate, 85-7°, 124-6° (from tetrahydrofuran-MeOH) [carbamate, m. 126-7° (from MeOH)]; β-alanylcetylamine hemihydrate, 84-6° (from Et2O), 124-6° (from dioxane-MeOH) [carbamate, m. 112-14° (from MeOH)]. N-Carbobenzyloxy-L-cysteinylstearylamine, m. 156-61° (from tetrahydrofuran) reduced with Na in liquid NH3 yielded 40% N-cysteinylstearylamine, m. 74-6°. N-Carbobenzyloxyaspartic acid anhydride (7.56 g.) in 35 cc. PhCH2OH treated 1 hr. with cooling with 1 equivalent PhCH2ONa yielded 7 g. PhCH2OCONHCH(OCOCH2Ph)CH2CO2H which condensed with IIa via the mixed anhydride with ClCO2Et gave the dicarbobenzyloxy derivative of N-stearyl-L-asparagine (XXXI), m. 92-4° (from MeOH); this treated with MeOH with H over Pd-C gave 60% XXXI, m. 168-70° (from MeOH). N-Carbobenzoyloxy-L-alanine condensed with L-alanylstearylamine followed by hydrogenolysis gave 80% L-alanyl-L-alanylstearylamine, m. 115-17° (from MeOH); N-carbobenzyloxy derivative, m. 163-4° (from tetrahydrofuran and MeOH). Similarly was prepared β-alanyl-β-alanylstearylamine monohydrate, m. 160-3°; carbobenzyloxy derivative, m. 175-8°. (CH2OH)2 (84 cc.), 1.5 g. Na, 20 g. C18H37Br, and 10 cc. tetrahydrofuran heated 96 hrs. at 120°, cooled, diluted with H2O, and extracted with Et2O gave 4.3 g. distearyl ether of (CH2OH)2, m. 55-7°; concentration of the mother liquors yielded 11.7 g. monostearyl ether (XXXII) of (CH2OH)2, white flaky solid, m. 51-2°. C18H37O(CH2)2CO2H (XXXIII) treated with LiAlH4 gave a product contaminated with C18H37OH (XXXIV). XXXIV (27 g.) added to 13 g. CH2:CHCO2Me in dry dioxane containing a trace of piperidine and PhCH2NMe3Br, the mixture refluxed overnight, concentrated, and diluted with H2O, the crude product washed with H2O and refluxed with 8 g. KOH in 500 cc. H2O, filtered, and acidified, the precipitate dissolved in Et2O, the solution treated with gaseous NH3, and the precipitate dissolved in H2O and acidified gave 4.5 g. XXXIII, m. 75-8° (from Et2O). XXXIII (1.7 g.) in dry tetrahydrofuran containing a trace Et3N treated at 0° with 0.5 cc. ClCO2Et, diluted after a few min. with absolute MeOH, and warmed to room temperature with stirring gave 1.7 g. Me ester of XXXIII, m. 53-6°, which was converted with concentrated NH4OH to the amide of XXXIII, m. 95-7° (from tetrahydrofuran-Et2O). The emulsion tests were carried out by dissolving the substance in 20 cc. H2O (employing generally the maximum concn), and mixing the solution in an Omnimixer with 5 cc. Nujol containing 0.2 g. cholesterol.

IT 59343-85-0P, Glucosamine, N-myristoyl- 911662-18-5P, Glucosamine, N-stearoyl-
RL: PREP (Preparation)
(preparation of)

RN 59343-85-0 CAPLUS

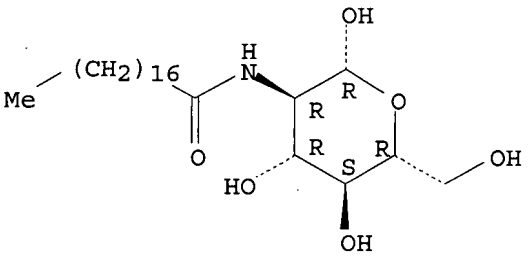
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxotetradecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 911662-18-5 CAPLUS
CN Glucosamine, N-stearoyl- (5CI) (CA INDEX NAME)

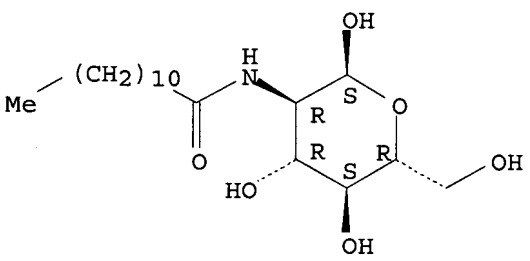
Absolute stereochemistry.



> d l15 1-9 ibib abs hitstr

L15 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:715470 CAPLUS
DOCUMENT NUMBER: 145:336305
TITLE: Design and synthesis of simple macrocycles active against vancomycin-resistant Enterococci (VRE)
AUTHOR(S): Jia, Yanxing; Ma, Nianchun; Liu, Zuosheng; Bois-Choussy, Michele; Gonzalez-Zamora, Eduardo; Malabarba, Adriano; Brunati, Cristina; Zhu, Jieping
CORPORATE SOURCE: Institut de Chimie des Substances Naturelles, CNRS, Gif-sur-Yvette, 91198, Fr.
SOURCE: Chemistry--A European Journal (2006), 12(20), 5334-5351
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 16-Membered meta,para-cyclophanes mimicking the vancomycin binding pocket (D-O-E ring) were designed and synthesized. The structural key features of these biaryl ether containing macrocycles are (1) the presence of β-amino-α-hydroxy acid or α,β-diamino acid as the C-terminal component of the cyclopeptide, and (2) the presence of a hydrophobic chain or lipidated aminoglucose at the appropriate position. Cycloetherification by an intramol. nucleophilic aromatic substitution reaction (SNAr) is used as the key step for the construction of the macrocycle. The atropselectivity of this ring-closure reaction is found to be sensitive to the peptide backbone and chemoselective cyclization (phenol vs. primary amine) is achievable. Glycosylation of phenol was realized with freshly prepared 3,4,6-tri-O-acetyl-2-N-lauroyl-2-amino-2-deoxy-α-D-glucopyranosyl bromide under phase-transfer conditions. Min. inhibitory concns. for all of the derivs. are measured by using a standard microdilution assay, and potent bioactivities against both sensitive and resistant strains are found for some of these compds. [MIC (min. inhibitory concentration) = 4 μg mL-1 against VRE]. From these preliminary SAR studies, it was anticipated that both the presence of a hydrophobic substituent and an appropriate structure of the macrocycle were required for this series of compds. to be active against VRE.
IT 909805-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of biaryl ether-containing glycosylated macrocycles, and their antibacterial activity against vancomycin-resistant Enterococci (VRE))
RN 909805-93-2 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[(1-oxododecyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 85 THERE ARE 85 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

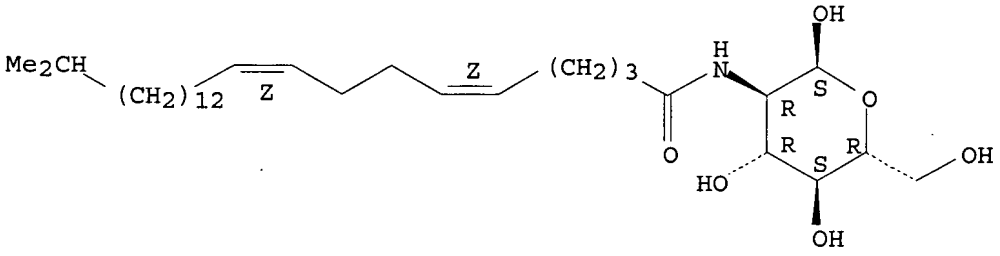
ACCESSION NUMBER: 2002:146451 CAPLUS
DOCUMENT NUMBER: 136:337921
TITLE: A new cytotoxic fatty acid (5Z,9Z)-22-methyl-5,9-tetracosadienoic acid and the sterols from the far eastern sponge Geodinella robusta
AUTHOR(S): Makarieva, Tatyana N.; Santalova, Elena A.; Gorshkova, Irina A.; Dmitrenok, Andrei S.; Guzii, Alla G.; Gorbach, Vladimir I.; Svetashev, Vassilii I.; Stonik, Valentin A.
CORPORATE SOURCE: Laboratory of the Marine Natural Products, Pacific Institute of Bioorganic Chemistry of the Russian Academy of Sciences, Vladivostok, 690022, Russia
SOURCE: Lipids (2002), 37(1), 75-80
CODEN: LPDSAP; ISSN: 0024-4201
PUBLISHER: AOCS Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new fatty acid, (5Z,9Z)-22-methyl-5,9-tetracosadienoic acid (I), and a rare fatty acid, (5Z,9Z)-23-methyl-5,9-tetracosadienoic acid (II), the predominant constituents of the free fatty acid fraction from the lipids of the sponge Geodinella robusta, were isolated and partly separated by reversed phase high-performance liquid chromatog., followed by multi-fold crystallization from MeOH to give I and II in 70% and 60% purity, resp. These fatty acids were identified as (5Z,9Z)-22- and (5Z,9Z)-23-methyl-5,9-tetracosadienoic acids by NMR techniques, including distortionless enhancement by polarization transfer, heteronuclear multiple quantum connectivity, and correlation spectroscopy expts., as well as from mass-spectrometric data for their Me esters, the Me esters of their perhydro derivs., and their pyrrolidides. Mixts. of I and II showed cytotoxic activity against mouse Ehrlich carcinoma cells and a hemolytic effect on mouse erythrocytes. The sterol fraction from the same sponge was analyzed by gas-liquid chromatog.-mass spectrometry, and 24-methylenecholesterol was identified as a main constituent of this fraction. The implications of the co-occurrence of membranolytic long-chain fatty acids and 24-methylenecholesterol as a main membrane sterol are discussed in terms of the phenomenon of biochem. coordination.

IT 415927-27-4P 416845-30-2P, N-[(5Z,9Z)-22-Methyl-5,9-tetracosadienoyl]-2-amino-α-D-glucopyranose
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)

RN 415927-27-4 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[[(5Z,9Z)-23-methyl-1-oxo-5,9-tetracosadienyl]amino]- (9CI) (CA INDEX NAME)

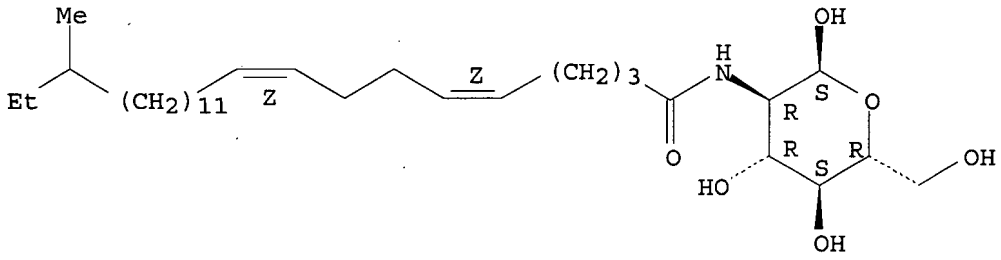
Absolute stereochemistry.
Double bond geometry as shown.



RN 416845-30-2 CAPLUS
CN α-D-Glucopyranose, 2-deoxy-2-[[(5Z,9Z)-22-methyl-1-oxo-5,9-tetracosadienyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

Currently available stereo shown.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

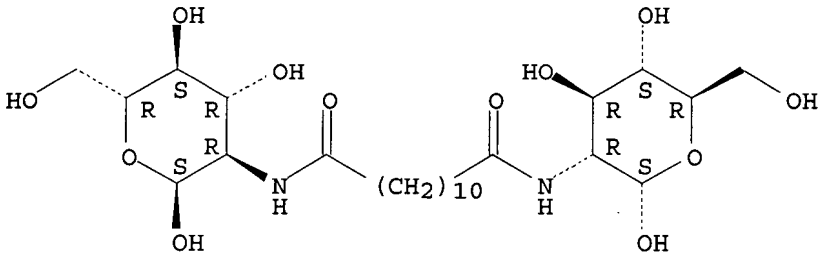
L15 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:426518 CAPLUS
DOCUMENT NUMBER: 131:228882
TITLE: Spontaneous Formation of Helically Twisted Fibers from 2-Glucosamide Bolaamphiphiles: Energy-Filtering Transmission Electron Microscopic Observation and Even-Odd Effect of Connecting Bridge
AUTHOR(S): Nakazawa, Ikuo; Masuda, Mitsutoshi; Okada, Yuji; Hanada, Takeshi; Yase, Kiyoshi; Asai, Michihiko; Shimizu, Toshimi
CORPORATE SOURCE: Joint Research Center for Precision Polymerization, Japan Chemical Innovation Institute, NIMC, and National Institute of Materials and Chemical Research, Tsukuba, Ibaraki, 305-8565, Japan
SOURCE: Langmuir (1999), 15(14), 4757-4764
CODEN: LANGD5; ISSN: 0743-7463
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of nonionic sugar-based bolaamphiphiles having n-alkylene chain length of 9, 10, 11, 12, 13, 14, 16, or 18 carbon atoms, N,N'-bis(2-deoxy-D-glucopyranoside-2-yl)alkane-1,n-dicarboxamide, 1(n), have been synthesized in one step from com. available glucosamine hydrochloride. Their self-assembling morphologies in 50% aqueous methanolic solns. have been studied using energy-filtering transmission electron microscopy (EF-TEM). The bolaamphiphiles 1(n) (n = 10, 12, and 14) with an even-numbered carbon bridge produced well-defined helically twisted fibers of 8-25 nm width with a high axial ratio. The fiber morphol. was found to display a pronounced even-odd dependence upon the number of carbons (n) in the connecting alkylene bridge. A similar trend was also exhibited by the IR band frequencies and by the wide-angle X-ray diffraction patterns. Anomeric ratios of 1(n) were approx. constant across the series and had no remarkable effect upon the fiber morphol.

IT 180073-74-9P 244070-32-4P 244070-33-5P
244070-34-6P 244070-35-7P 244070-36-8P
244070-37-9P 244070-38-0P 244070-39-1P
244070-40-4P 244070-41-5P 244070-42-6P
244070-43-7P 244070-44-8P 244070-45-9P
244070-46-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(spontaneous formation of helically twisted fibrous structures in glucosamide bolaamphiphiles)

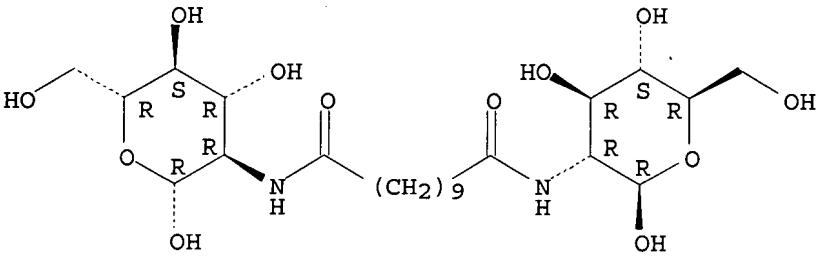
RN 180073-74-9 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,12-dioxo-1,12-dodecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



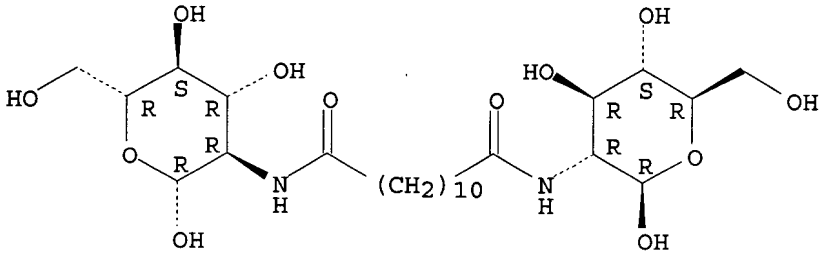
RN 244070-32-4 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,11-dioxo-1,11-undecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



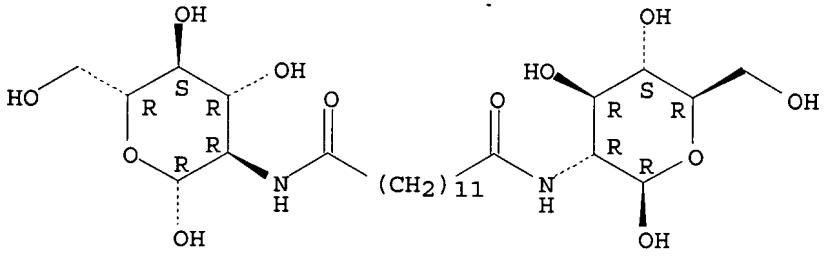
RN 244070-33-5 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,12-dioxo-1,12-dodecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244070-34-6 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,13-dioxo-1,13-tridecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

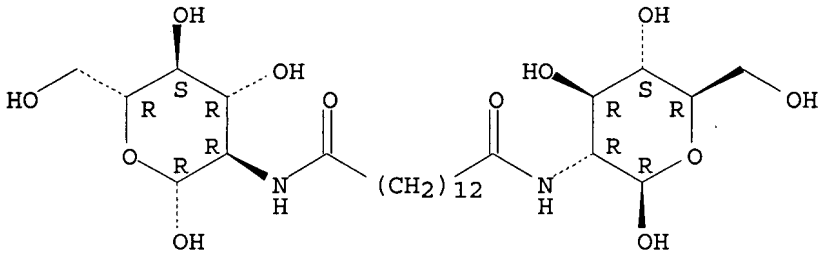
Absolute stereochemistry.



RN 244070-35-7 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,14-dioxo-1,14-

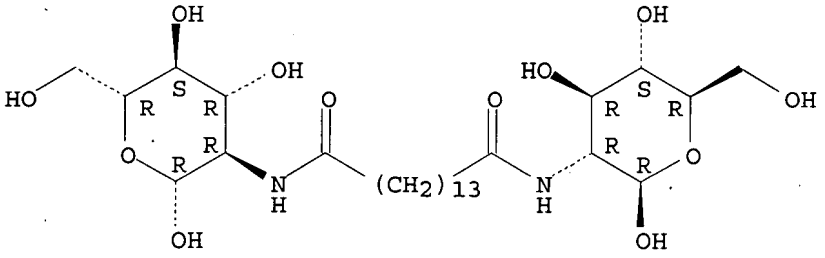
tetradecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



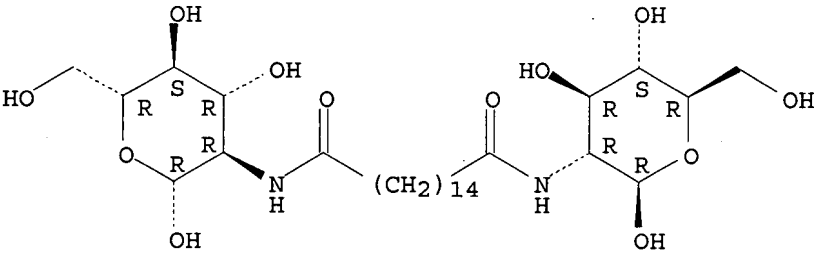
RN 244070-36-8 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,15-dioxo-1,15-pentadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



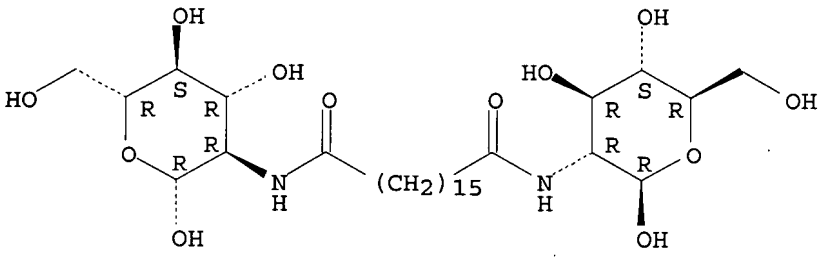
RN 244070-37-9 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,16-dioxo-1,16-hexadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



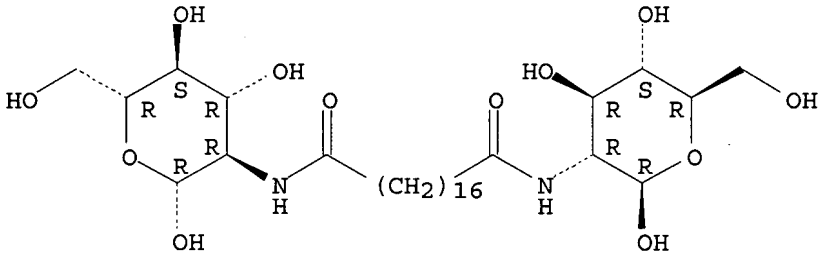
RN 244070-38-0 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,17-dioxo-1,17-heptadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



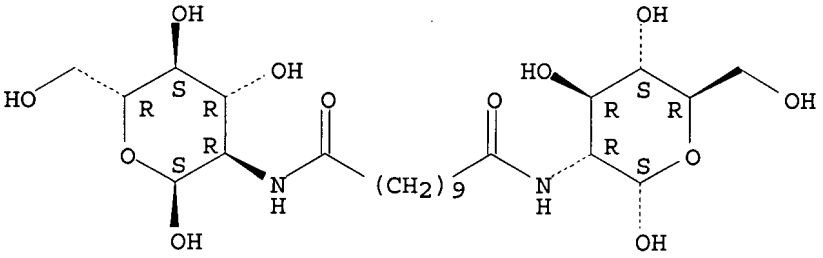
RN 244070-39-1 CAPLUS
CN β-D-Glucopyranose, 2,2'-[(1,18-dioxo-1,18-octadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



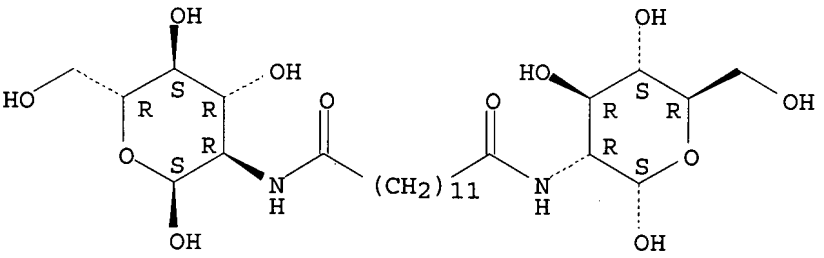
RN 244070-40-4 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,11-dioxo-1,11-undecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



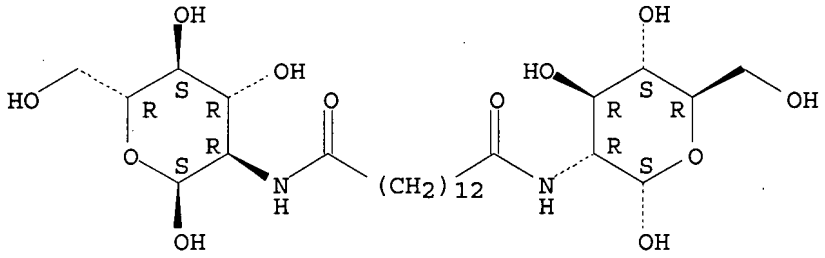
RN 244070-41-5 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,13-dioxo-1,13-tridecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



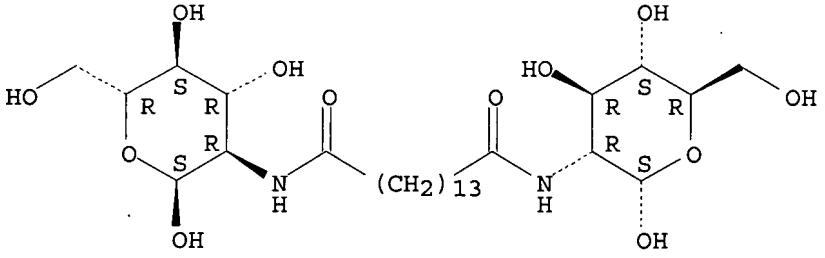
RN 244070-42-6 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,14-dioxo-1,14-tetradecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



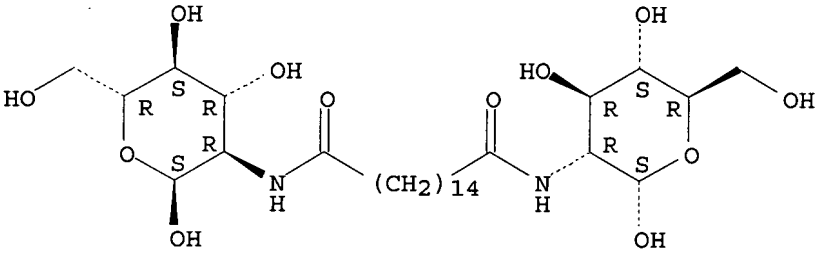
RN 244070-43-7 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,15-dioxo-1,15-pentadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



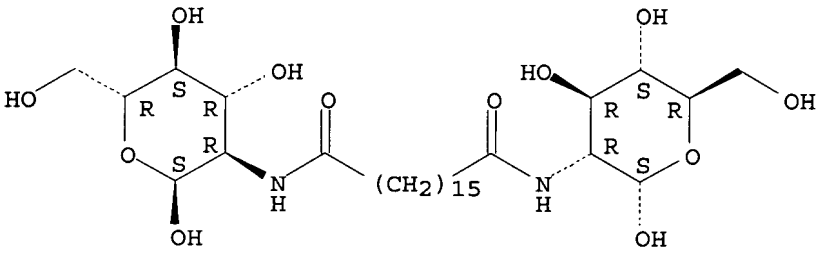
RN 244070-44-8 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,16-dioxo-1,16-hexadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 244070-45-9 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,17-dioxo-1,17-heptadecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

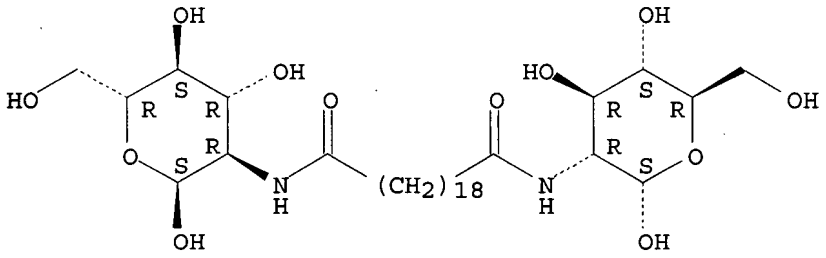
Absolute stereochemistry.



RN 244070-46-0 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,20-dioxo-1,20-eicosanediyl)diimino]bis[2-

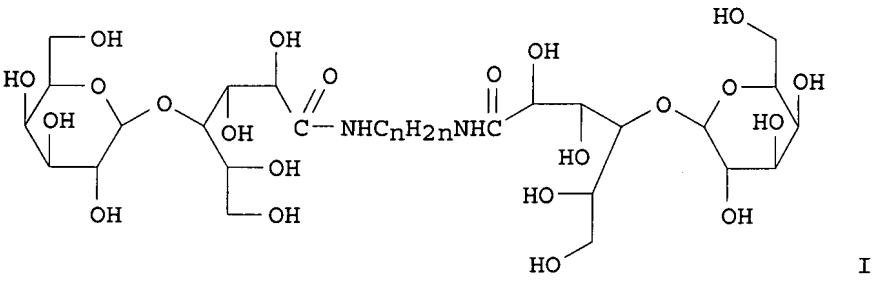
deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:392909 CAPLUS
DOCUMENT NUMBER: 125:168516
TITLE: Synthesis of new sugar-based bolaamphiphilic compounds. Physicochemical study of their molecular aggregation in aqueous solution
AUTHOR(S): Brisset, F.; Garelli-Calvet, R.; Azema, J.; Chebli, C.; Rico-Lattes, I.; Lattes, A.; Moisand, A.
CORPORATE SOURCE: Lab. IMRCP, Univ. Paul Sabatier, Toulouse Cedex, 31062, Fr.
SOURCE: New Journal of Chemistry (1996), 20(5), 595-605
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Gauthier-Villars
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



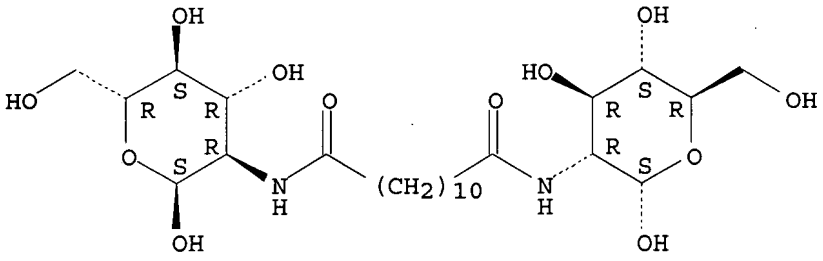
I

AB The synthesis of new sugar-based bolaamphiphiles, e.g. I (n = 6, 7), is reported. The sugar-based polar heads were mono- or diholosides in either the open or closed configuration. Micellization was shown to occur with compds. whose alkyl chain length was above a certain value. Aggregation in micelles was assumed to be the result of chain folding. For compds. with short alkyl chains, vesicles were obtained under certain conditions. These new synthetic bolaforms may find applications in drug formulation to solubilize hydrophobic compds. such as fatty acids. The globular systems formed do not denature lipoxygenase-type enzymes. The activity of soybean lipoxygenase was examined in the presence of the different bolaforms synthesized and compared to that observed in the presence of Tween 20.

IT 180073-74-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

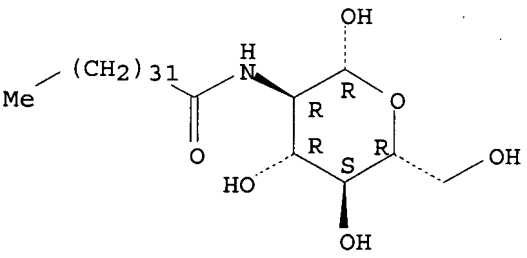
(synthesis of new sugar-based bolaamphiphiles)
RN 180073-74-9 CAPLUS
CN α-D-Glucopyranose, 2,2'-[(1,12-dioxo-1,12-dodecanediyl)diimino]bis[2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



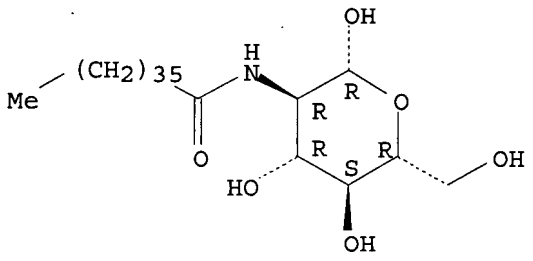
L15 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:170112 CAPLUS
DOCUMENT NUMBER: 116:170112
TITLE: Studies on the constituents of Ganoderma applanatum
AUTHOR(S): Chiang, Hung Cheh; Ho, Chiao Ching
CORPORATE SOURCE: Inst. Chem., Natl. Taiwan Norm. Univ., Taipei, Taiwan
SOURCE: Huaxue (1990), 48(4), 253-8
CODEN: HUHSA2; ISSN: 0441-3768
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Seven compds. [ergosta-7,22-dien-3β-yl-palmitate, alnusenone, fridelin, ergosta-7,22-dien-3-one, ergosta-7,22-dien-3β-ol, ergosterol, ergosta-5,8,22-trien-3β,15-diol] are identified from Ganoderma applanatum. Two kinds of mixed crystals [ergosterol peroxide and 9(11)-dehydroergosterol peroxide mixture, long chain(C32-C36) carboxylate of glucosamine mixture are separated
IT 139595-18-9
RL: BIOL (Biological study)
(from Ganoderma applanatum)
RN 139595-18-9 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxotritriacontyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



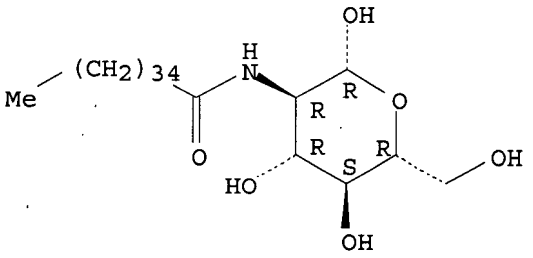
IT 139595-31-6P 139595-32-7P 139595-33-8P
139984-96-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 139595-31-6 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxoheptatriacontyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



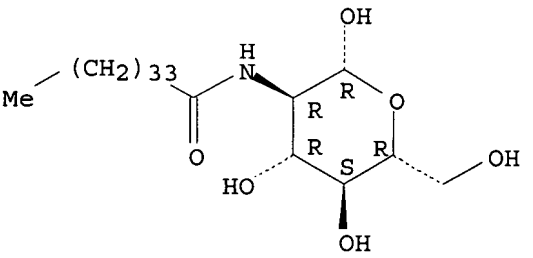
RN 139595-32-7 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxohexatriacontyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



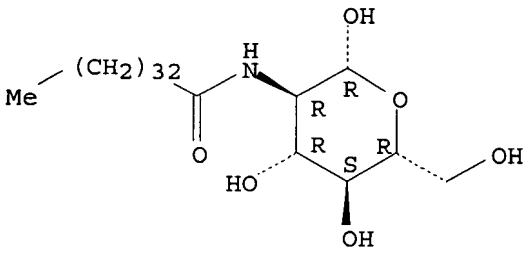
RN 139595-33-8 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxopentatriacontyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 139984-96-6 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(1-oxotetratriacontyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

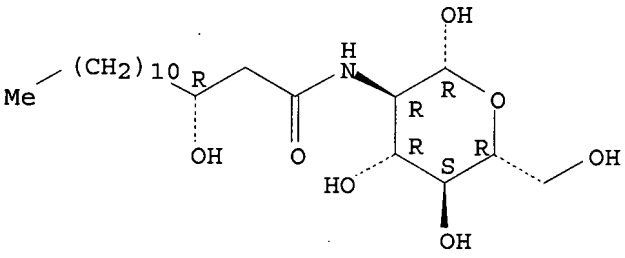


L15 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:4713 CAPLUS
DOCUMENT NUMBER: 114:4713
TITLE: Specific binding of lipopolysaccharides to mouse macrophages. II. Involvement of distinct lipid A substructures
AUTHOR(S): Tahri-Jouti, Mohamed Ali; Mondange, Michelle; Le Dur, Annick; Auzanneau, France Isabelle; Charon, Daniel; Girard, Robert; Chaby, Richard
CORPORATE SOURCE: Unite Rech. Associee, Univ. Paris-Sud, Orsay, 91405, Fr.
SOURCE: Molecular Immunology (1990), 27(8), 763-70
CODEN: MOIMD5; ISSN: 0161-5890
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interaction of lipopolysaccharide-binding sites of mouse macrophages with the lipid A region of endotoxins (LPS) was demonstrated by direct binding of labeled lipid A conjugates, by inhibition of the binding of labeled LPS with anti-lipid A monoclonal antibodies, and by the considerable reduction of this binding after chemical and enzymic removal of the fatty acid esters of the LPS. The substructures of lipid A required for the specific binding of LPS to macrophages were analyzed by the use of synthetic lipids consisting of mono- or disaccharide derivs. of glucosamine. The two phosphate groups of lipid A (at positions 1 and 4') as well as certain hydroxyl groups, appeared to play a critical role in the binding. However, the reactivities of the synthetic lipids with the macrophage surface, as compared with those with anti-lipid A antibodies, could hardly be explained by the existence of a single LPS receptor, and suggested the presence, on the macrophage surface, of different LPS-binding sites that recognize different substructures or spatial configurations of the lipid moiety of endotoxins.

IT 96151-64-3
RL: BIOL (Biological study)
(as lipid A analog, macrophage binding to, lipopolysaccharide receptor in relation to)
RN 96151-64-3 CAPLUS
CN β-D-Glucopyranose, 2-deoxy-2-[(3-hydroxy-1-oxotetradecyl)amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:119509 CAPLUS
DOCUMENT NUMBER: 112:119509
TITLE: Synthesis and liquid-crystalline behavior of liposaccharide based comb polymers
AUTHOR(S): Gallot, Bernard; Marchin, Brigitte
CORPORATE SOURCE: Cent. Biophys. Mol., CNRS, Orleans, 45071, Fr.
SOURCE: Liquid Crystals (1989), 5(6), 1729-35
CODEN: LICRE6; ISSN: 0267-8292
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Liquid-crystalline homopolymers were prepared from 11-(acryloylamino)undecanoyl-N-methylglucamine, 11-(acryloylamino)undecanoylaminogalactose, or 11-(acryloylamino)undecanoylaminoglucose. The polymers exhibited mesophases in concentrated aqueous, EtOH, or DMSO solution, and the mesomorphic character remained after slow evaporation of the solvent. The mesophases had smectic or nematic ordering depending on the saccharide residue.

IT 125863-55-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(liquid-crystalline, preparation and properties of)

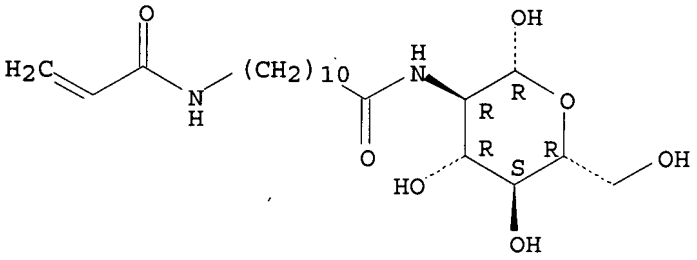
RN 125863-55-0 CAPLUS

CN β-D-Glucopyranose, 2-deoxy-2-[[1-oxo-11-[(1-oxo-2-propenyl)amino]undecyl]amino]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

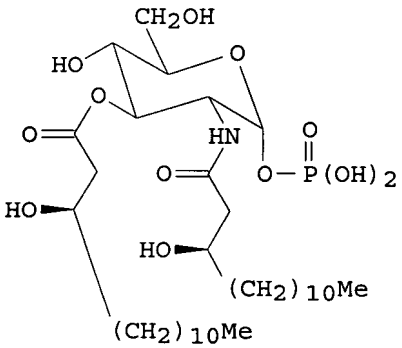
CRN 125863-54-9
CMF C20 H36 N2 O7

Absolute stereochemistry.



L15 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:22186 CAPLUS
DOCUMENT NUMBER: 108:22186
TITLE: A convenient synthesis of 2-deoxy-2-[(R)-3-hydroxytetradecanamido]-3-O-[(R)-3-hydroxytetradecanoyl]-α-D-glucopyranose 1-phosphate (lipid X)
AUTHOR(S): Macher, Ingolf
CORPORATE SOURCE: Sandoz Forschungsinst., Vienna, A-1235, Austria
SOURCE: Carbohydrate Research (1987), 162(1), 79-84
CODEN: CRBRAT; ISSN: 0008-6215
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:22186
GI



I

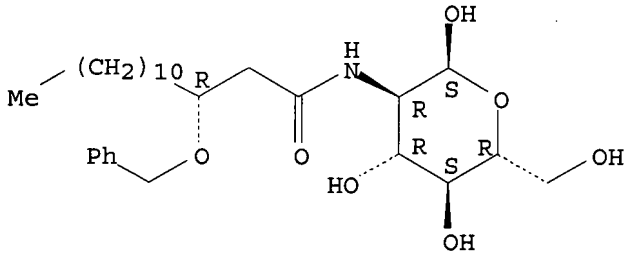
AB The crystalline tris(hydroxymethyl)aminomethane (Tris) salt of lipid X (I) was synthesized from 2-amino-2-deoxy-D-glucose hydrochloride in five steps in .apprx.50% overall yield. The key step was 1-O-(dibenzyl)phosphorylation of 4,6-O-benzylidene-2-[(R)-3-benzyloxytetradecanamido]-2-deoxy-D-glucopyranose, catalyzed by BuLi. The product was then 3-(R)-3-benzyloxytetradecanoylated, and the benzyl and benzylidene groups were removed by catalytic hydrogenolysis.

IT 111789-76-5P 111789-79-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and benzyldenation of)

RN 111789-76-5 CAPLUS

CN α-D-Glucopyranose, 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, (R)- (9CI) (CA INDEX NAME)

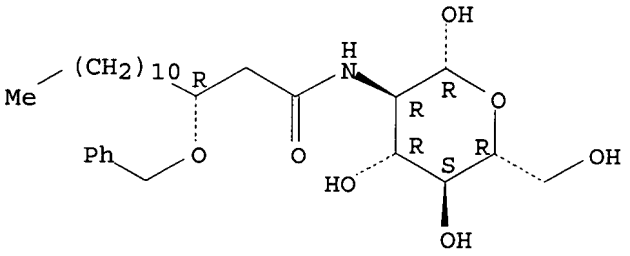
Absolute stereochemistry.



RN 111789-79-8 CAPLUS

CN β-D-Glucopyranose, 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L15 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:103706 CAPLUS

DOCUMENT NUMBER: 104:103706

TITLE: Lipid A monosaccharide analogs inhibiting oxidative phosphorylation

AUTHOR(S): Gillois, M.; Silve, G.; Asselineau, J.; Laneelle, G.

CORPORATE SOURCE: Cent. Rech. Biochim. Genet. Cell., Univ. Paul Sabatier, Toulouse, 31062, Fr.

SOURCE: Annales de l'Institut Pasteur/Microbiology (1985), 136B(2), 125-34
CODEN: AIPME3; ISSN: 0769-2609

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Three acyl-glucosamine analogs of lipid A and an acyl-glucose analog of cord factor were synthesized and their activity was tested on isolated rat liver mitochondria. The 4 glycolipids slightly inhibited succinate-supported active respiration and strongly inhibited glutamate-supported active respiration. The most potent inhibitors were

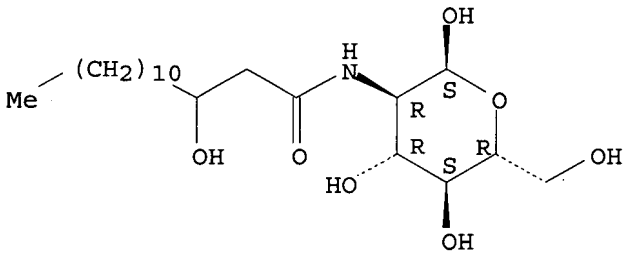
the 2 diacylated compds. which are the most hydrophobic. Phosphorylation was also impaired. Comparison of the results with the few published data about the effects of lipid A on mitochondria indicated that the 2 diacylated glucosamines were as active as their natural model. The minimal requirements to obtain a glycolipid structure with an activity resembling that of lipid A is discussed.

IT 100680-91-9
RL: BIOL (Biological study)
(oxidative phosphorylaiton by liver mitochondria response to)

RN 100680-91-9 CAPLUS

CN α-D-Glucopyranose, 2-deoxy-2-[(3-hydroxy-1-oxotetradecyl)amino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



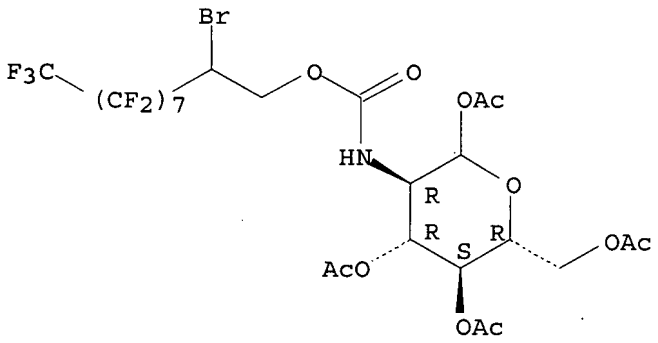
L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:106066 CAPLUS
DOCUMENT NUMBER: 144:350955
TITLE: Froc: A New Fluorous Protective Group for Peptide and Oligosaccharide Synthesis
AUTHOR(S): Manzoni, Leonardo; Castelli, Riccardo
CORPORATE SOURCE: Centro Interdisciplinare Studi Biomolecolari e applicazioni Industriali (CISI), C.N.R. - Istituto di Scienze e Tecnologie Molecolari (ISTM), Milan, I-20133, Italy
SOURCE: Organic Letters (2006), 8(5), 955-957
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:350955

AB The synthesis of a new fluorous protecting group, Froc, C8F17CH(Br)CH2OCO, is described. The authors have used this new fluorous tag, in the form of Froc-Cl, in peptide and carbohydrate synthesis, where each product was fully characterized by NMR and MS, and each step was monitored by TLC. Purification of the products is generally performed by standard fluorous solid-phase extraction techniques (e.g., F-SPE), but standard chromatog. purifications are also possible if required.

IT 881425-80-5P 881425-82-7P 881425-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorous protective group "Froc" for uses in peptide and oligosaccharide synthesis)

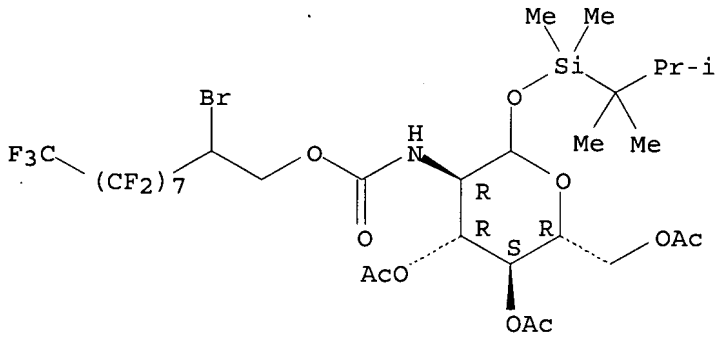
RN 881425-80-5 CAPLUS
CN D-Glucopyranose, 2-[[[(2-bromo-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)oxy]carbonyl]amino]-2-deoxy-, 1,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



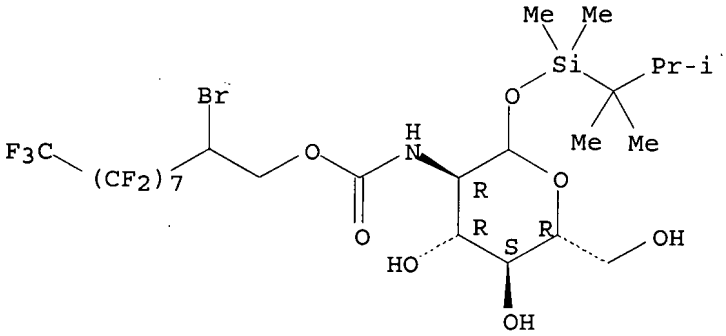
RN 881425-82-7 CAPLUS
CN D-Glucopyranose, 2-[[[(2-bromo-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)oxy]carbonyl]amino]-2-deoxy-1-O-[dimethyl(1,1,2-trimethylpropyl)silyl]-, 3,4,6-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 881425-83-8 CAPLUS
CN D-Glucopyranose, 2-[[[(2-bromo-3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)oxy]carbonyl]amino]-2-deoxy-1-O-[dimethyl(1,1,2-trimethylpropyl)silyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

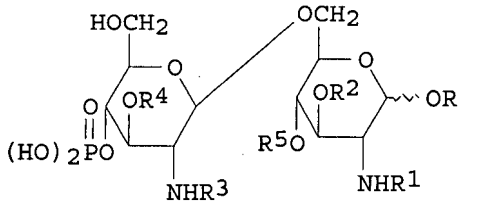


REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:552973 CAPLUS
DOCUMENT NUMBER: 113:152973
TITLE: Preparation of 6-O-(β-D-glucosaminyl)-D-glucosamine phosphate derivatives as antitumor agents
INVENTOR(S): Shiba, Tetsuo; Soga, Tsunehiko; Kusama, Tsuneom
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Pat. Specif. (Aust.), 121 pp.
CODEN: ALXXAP
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
AU 595987	B2	19900412	AU 1988-12541	19880301
AU 8812541	A	19890907		
PRIORITY APPLN. INFO.:			AU 1988-12541	19880301

OTHER SOURCE(S): MARPAT 113:152973
GI



I

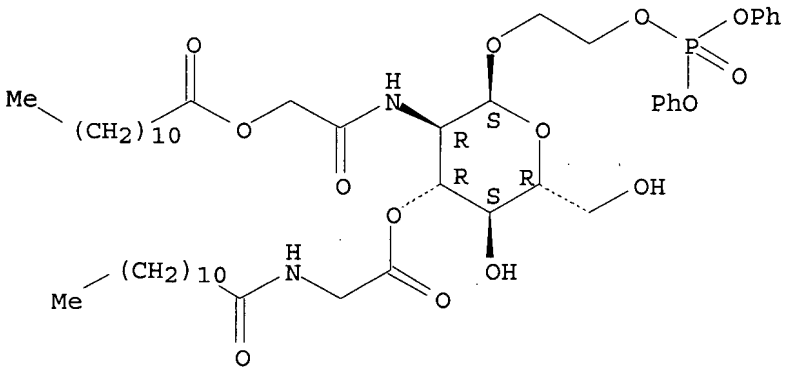
AB The title disaccharide derivs. [I; R = P(O)(OH)2, ZR6, CH(Z1R6)Z2R6; Z, Z1, Z2 = C1-6 alkylene; R6 = CO2H, P(O)(OH)2; R1, R2, R3, R4 = COR7, COZ3R8, CO(CH2)lCHQNQ1COR7, CO(CH2)lCHQNQ1COZ3R8, CO(CH2)mO2CR7, CO(CH2)mO2CZ3R8, CO(CH2)mCOR7, CO(CH2)mCOZ3R8, CO(CH2)mCOC(CH2)nNQ1COR7, CO(CH2)mCO(CH2)nNQ1COZ3R8; R7 = (un)substituted C1-30 alkyl; Z3 = C1-9 alkylene; R8 = C3-12 (one or more HO-substituted) cycloalkyl; Q = H, C1-6 alkyl, CONH2, CO2H, CH2OH; Q1 = H, C1-20 alkyl; l = 0-20; m, n = 1-20; R5 = H, P(O)(OH)2, CO(CH2)pCO2H; p = 1-6; excluding a combination of R = P(O)(OH)2, R5 = H, R1 = R2 = R3 = R4 = COR7] which are lipid A analogs having antitumor activity equal to or higher than that of the known lipid A analog I [R = P(O)(OH)2, R1, R2 = (R)-3-hydroxytetradecanoyl, R3 = (R)-3-dodecanoyloxytetradecanoyl, R4 = (R)-4-tetradecanoyloxytetradecanoyl , R5 = H] (II) and lower toxicity than II, are prepared Thus, I [OR = α-CH2CH2P(O)(OH)2, R1, R3 = N-dodecanoyl-N-methylglyclyl, R2, R4 = N-dodecanoylglycyl, R5 = H] (III) was prepared by bromination of 1-O-acetyl-2-deoxy-4-O-diphenylphosphono-3-O-(N-dodecanoylglycyl)-6-O-(2,2,2-trichloroethoxycarbonyl)-2-(2,2,2-trichloroethoxycarbonylamino)-D-glucopyranose followed by glycosidation with 2-(diphenylphosphonoxy)ethyl 2-deoxy-3-O-(N-dodecanoylglycyl)-2-[(N-dodecanoyl-N-methylglycyl)amino]-α-D-glucopyranoside and deprotection of the trichloroethoxy carbonyl group with Zn powder from the resulting glycoside followed by N,O-acylation with N-dodecanoyl-N-methylglycine and hydrogenolysis. A total of 81 I were prepared and III administered to the mice at 100 μg/mouse i.v. on the 7th, 12th, and 21st days from the implantation of fibrosarcoma cells, inhibited tumor growth by 19%, vs. 15% for II.

IT 123574-38-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor lipid A analog)

RN 123574-38-9 CAPLUS

CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-[(diphenoxyphosphinyl)oxy]ethyl 2-deoxy-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

Absolute stereochemistry.

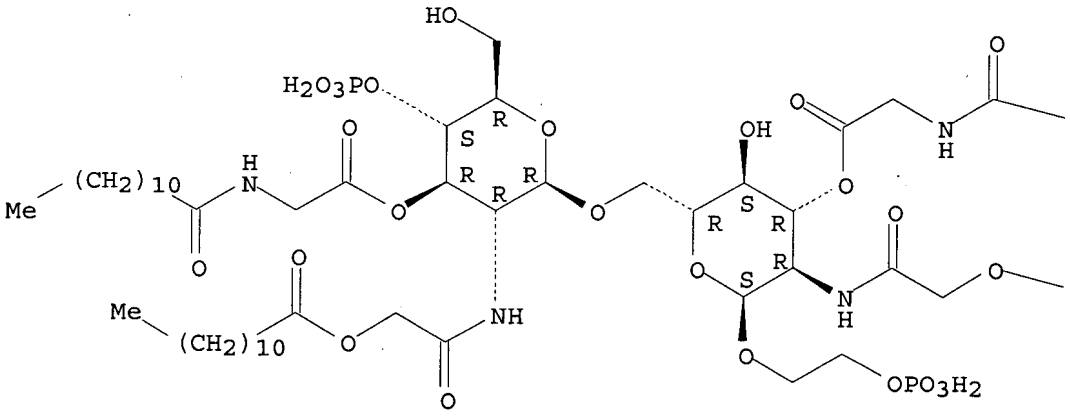


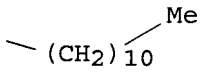
IT 123598-15-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antitumor lipid A analog)

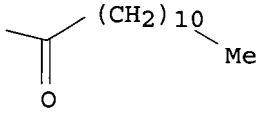
RN 123598-15-2 CAPLUS

CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-(phosphonooxy)ethyl 2-deoxy-6-O-[2-deoxy-3-O-[[(1-oxododecyl)amino]acetyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-4-O-phosphono-β-D-glucopyranosyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

Absolute stereochemistry.



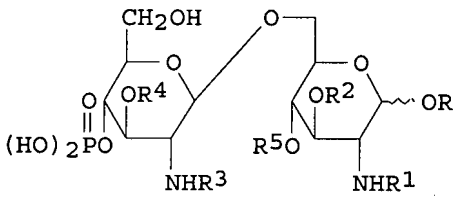




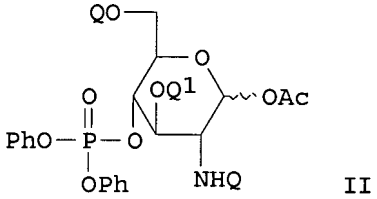
L23 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:198980 CAPLUS
DOCUMENT NUMBER: 112:198980
TITLE: Preparation of amino disaccharides as antitumor agents
INVENTOR(S): Kusama, Tsuneo; Soga, Tsunehiko; Shiba, Tetsuo
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 81 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 330715	A1	19890906	EP 1988-103185	19880302
EP 330715	B1	19930616		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
US 5006647	A	19910409	US 1988-162932	19880302
AT 90685	T	19930715	AT 1988-103185	19880302
CA 1320951	C	19930803	CA 1988-560369	19880302
US 5134230	A	19920728	US 1991-614417	19910118
PRIORITY APPLN. INFO.:			EP 1988-103185	19880302
			US 1988-162932 A3	19880302

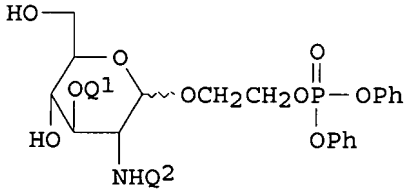
OTHER SOURCE(S): CASREACT 112:198980; MARPAT 112:198980
GI



I



II



III

AB The title compds. [I; R = P(O)(OH)2, ZR6, CH(Z1R6)Z2R6; R1, R2, R3, R4 = COR7, COZ3R8, etc.; R5 = H, phosphono, CO(CH2)mCO2H; R6 = CO2H, OP(O)(OH)2; R7 = alkyl; R8 = (substituted) cycloalkyl; Z, Z1, Z2, Z3 = alkylene; m = 0, 1-6 integer], useful for treatment of immunodeficiency, infectious, and neoplastic diseases, are prepared Glucopyranose derivative II [Q = CO2CH2CCl3; Q1 = COCH2NHCO(CH2)10Me] in CH2Cl2 was treated with HBr in HOAc and the product condensed with phosphonoethyl glucopyranoside III [Q2 = COCH2NMeCO(CH2)10Me] to give I [R = CH2CH2OP(O)(OPh)2; R1 = Q2; R2 = R4 = Q1; R3 = Q; R5 = H], which in HOAc was treated with Zn, and the product acylated with HOQ2 in THF containing 1-hydroxybenzotriazole to give I [R = CH2CH2OP(O)(OPh)2; R1 = R3 = Q2; R2 = R4 = Q1; R5 = H]. Hydrogenolysis of this over PtO2 gave I [R = CH2CH2OP(O)(OH)2; R1 = R3 = Q2; R2 = R4 = Q1; R5 = H]. This showed a 19% suppression of tumor growth against fibrosarcoma cells (Meth A) implanted in BALB-c mice vs. 15% for natural lipid A.

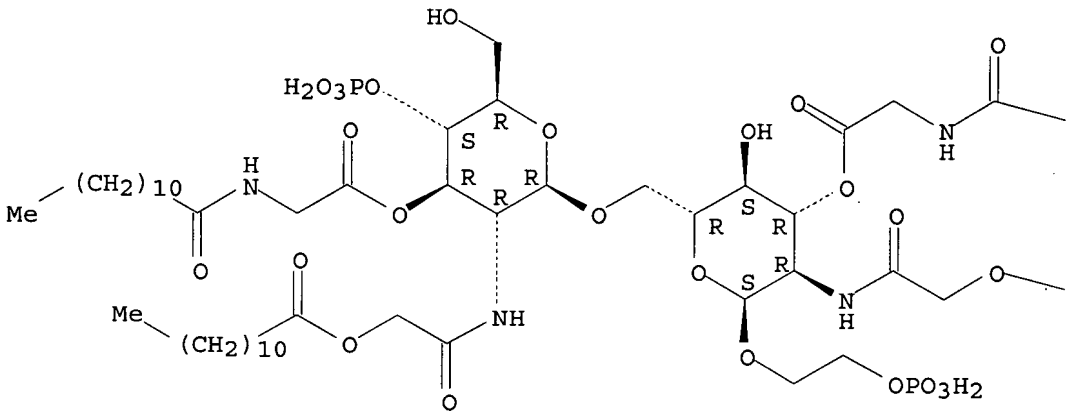
IT 123598-15-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)

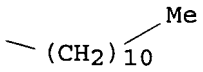
RN 123598-15-2 CAPLUS

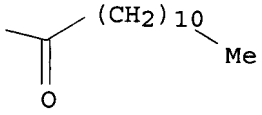
CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-(phosphonooxy)ethyl 2-deoxy-6-O-[2-deoxy-3-O-[[(1-oxododecyl)amino]acetyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-4-O-phosphono-β-D-glucopyranosyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

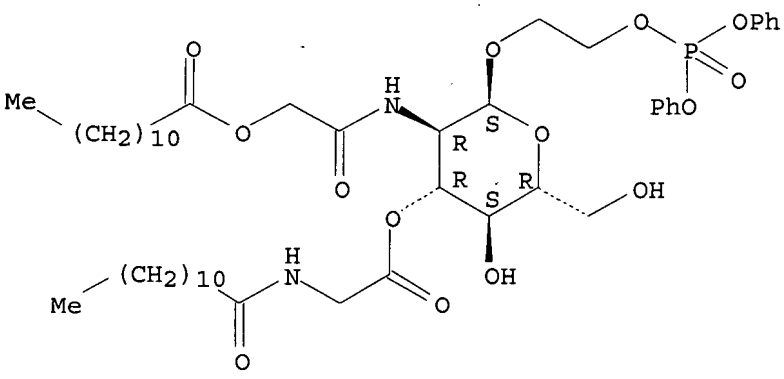






IT 123574-38-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for drugs)
RN 123574-38-9 CAPLUS
CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-[(diphenoxyphosphinyl)oxy]ethyl 2-deoxy-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

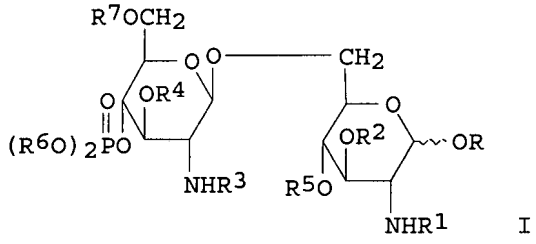
Absolute stereochemistry.



L23 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:99142 CAPLUS
DOCUMENT NUMBER: 112:99142
TITLE: Preparation of 6-O-(β-D-glucosaminyl)glucosamine derivatives as antitumor agents
INVENTOR(S): Nichima, Tsuneo; Soga, Tsunehiko
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 43 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01221387	A	19890904	JP 1988-47247	19880229
JP 2535048	B2	19960918		
PRIORITY APPLN. INFO.:			JP 1988-47247	19880229

OTHER SOURCE(S): MARPAT 112:99142
GI



I

AB Disaccharide derivs. [I; R = P(O)(OH)2, ZR8, CH(Z1R8)Z2R8; Z - Z2 = C1-6 alkylene; R8 = CO2H, OP(O)(OH)2; R1-R4 = COR9, COZ3R10, CO(CH2)nCHQNQ1COR9, CO(CH2)nCHQNQ1COZ3R10, etc.; R9 = straight chain or branched C1-30 alkyl optionally substituted by ≥1 OH; Z3 = C1-9 alkylene; R6 = R7 = H; R10 = C3-12 cycloalkyl optionally substituted by ≥1 OH; Q = C1-6 alkyl, CONH2, CO2H, CH2OH; Q1 = H, C1-20 alkyl; n = 0-10; R5 = H, (HO)2P(O), CO(CH2)mCO2H; m = 0-5; excluding a combination of R = P(O)(OH)2 or ZR8, R5 = H or P(O)(OH)2, and R1-R4 = COR9], useful as antitumor agents with reduced toxicity compared to the known lipid A analog I [R = P(O)(OH)2, R1 = R2 = (R)-3-hydroxytetradecanoyl, R3 = (R)-3-dodecanoyloxytetradecanoyl, R4 = (R)-3-tetradecanoyloxytetradecanoyl , R5 - R7 = H] II), are prepared Thus, treatment of 1-O-acetyl-2-deoxy-4-O-diphenylphosphono-3-O-(N-dodecanoylglycyl)-6-O-(2,2,2-trichloroethoxycarbonyl)-2-(2,2,2-trichloroethoxycarbonylamino)-D-glucose with 25% HBr/AcOH in CH2Cl2 followed by glycosidation with 2-(diphenylphosphonoxyl)ethyl 2-deoxy-3-O-(N-dodecanoylglycyl)-2-[(N-dodecanoyl-N-methylglycyl)amino]-α-D-glucopyranoside in the presence of activated CaSO4 and Hg(CN)2 in CH2Cl2 at 50-60° gave I [OR = α-OCH2CH2OP(O)(OPh)2, R1 = N-dodecanoyl-N-methylglycyl, R2 = R4 = N-dodecanoylglycyl, R3 = R7 = Cl3CCH2O2C, R5 = H, R6 = Ph] which was deprotected with Zn in AcOH and then condensed with N-dodecanoyl-N-methylglycine in THF in the presence of 1-hydroxybenzotriazole and DCC to give, after hydrogenolysis over PtO2 in THF, I [OR = α-OCH2CH2OP(O)(OH)2, R1 = R3 = N-dodecanoyl-N-methylglycyl, R2 = R4 = N-dodecanoylglycyl, R5-R7 = H] (III). III and I [OR = α-OCH2CH2OP(O)(OH)2, R1 = R3 = N-dodecanoyl-N-dodecylglycyl, R2 = R4 = N-dodecanoylglycyl, R5-R7 = H] inhibited 19 and 24%, resp., the growth of fibroblast sarcoma Meth A transplated in mice vs. 15% for II.

IT 123598-15-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antitumor agent)

RN 123598-15-2 CAPLUS

CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-(phosphonooxy)ethyl 2-deoxy-6-O-[2-deoxy-3-O-[[(1-oxododecyl)amino]acetyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-4-O-phosphono-β-D-glucopyranosyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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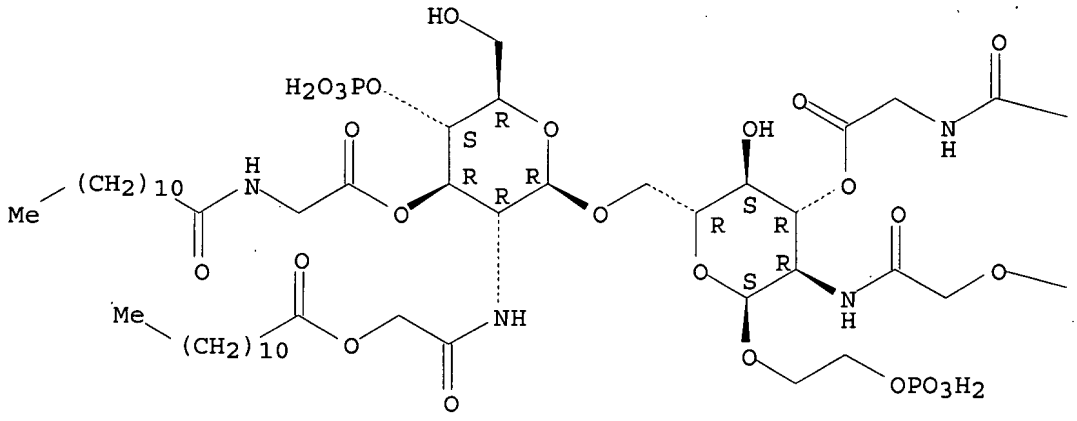
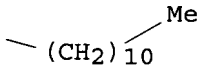
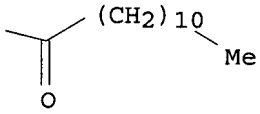


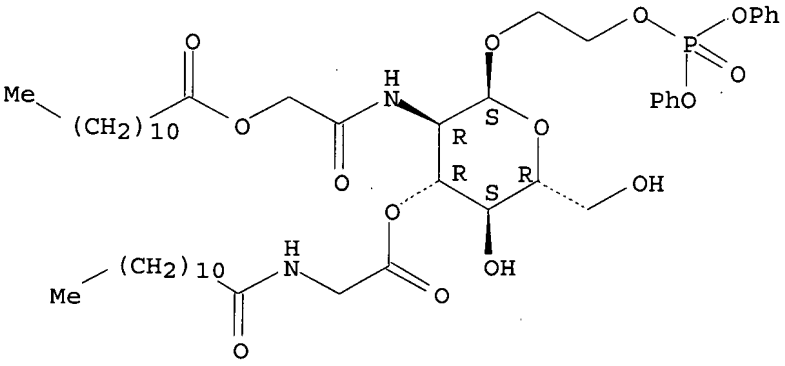
PAGE 1-B





IT 123574-38-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antitumor agent)
RN 123574-38-9 CAPLUS
CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-[(diphenoxyphosphinyl)oxy]ethyl 2-deoxy-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

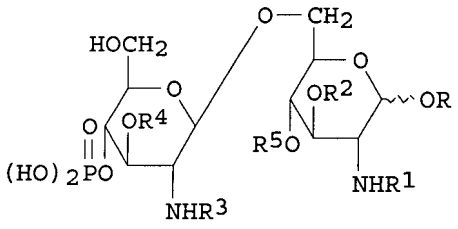
Absolute stereochemistry.



L23 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:77859 CAPLUS
DOCUMENT NUMBER: 112:77859
TITLE: Preparation and testing of N,O-acyldiglucosamine phosphates as antitumor agents
INVENTOR(S): Kusama, Tsuneo; Soga, Tsunehiko; Shiba, Tetsuo
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: S. African, 117 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 8801430	A	19881228	ZA 1988-1430	19880229

PRIORITY APPLN. INFO.: ZA 1988-1430 19880229
OTHER SOURCE(S): MARPAT 112:77859
GI



I

AB The title disaccharides [I; R = (HO)2P(O), CH(Z1R6)Z2R6; Z, Z1, Z2 = C1-6 alkylene; R6 = CO2H, OP(O)(OH)2; R1-R4 = COR7, COZ3R8, CO(CH2)lCHQNQ1COR7, CO(CH2)lCHQNQ1COZ3R8, CO(CH2)mCOR7, CO(CH2)mO2CZ3R8, CO(CH2)mCOR7, CO(CH2)mCOZ3R8, CO(CH2)mCO(CH2)mNQ1COR7, CO(CH2)mCO(CH2)nNQ1COZ3R8; R7 = C1-30 alkyl optionally substituted with ≥1 OH groups; Z3 = C1-9 alkylene; R8 = C3-12 cycloalkyl optionally substituted with ≥1 OH groups; Q = H, C1-6 alkyl, CONH2, CO2H, CH2OH; Q1 = H, C1-20 alkyl; l, m, n, = 0-20; R5 = H, (HO)2P(O), HO2C(CH2)oCO; o = 0-6; excluding a combination wherein R = (HO)2P(O), R5 = H, and R1-R4 = COR7] useful as antitumor agents, were prepared Bromination of 1-O-acetyl-2-deoxy-4-O-diphenylphosphono-3-O-(N-dodecanoylglycyl)-6-O-(2,2,2-trichloroethoxycarbonyl)-2-(2,2,2-trichloroethoxycarbonyl)-D-glucopyranose with a CH2Cl2 solution of 30% HBr in AcOH followed by glycosidation with 2-(diphenylphosphonoxy)ethyl 2-deoxy-3-O-(N-dodecanoylglycyl)-2-[(N-dodecanoyl-N-methylglycyl)amino]-α-D-glucopyranoside in CH2Cl2 in the presence of activated CaSO4 and Hg(CN)2 gave 2-(diphenylphosphonoxy)ethyl 2-deoxy-6-O-[2-deoxy-4-O-diphenylphosphono-3-O-(N-dodecanoylglycyl)-6-O-(2,2,2-trichloroethoxycarbonyl)-2-(2,2,2-trichloroethoxycarbonylamino-β-D-glucopyranosyl]-3-O-(N-dodecanoylglycyl)-2-[(N-dodecanoyl-N-methylglycyl)amino]-α-D-glucopyranoside. Deprotection of the latter with Zn powder in AcOH followed by amidation with N-dodecanoyl-N-methylglycine in THF containing DCC and 1-hydroxybenzotriazole and hydrogenolysis over PtO2 in THF gave I [R = α-CH2CH2OP(O)(OH)2, R1 = R3 = N-dodecanoyl-N-methylglycyl, R2 = R4 = N-dodecanoylglycyl, R5 = (HO)2P(O)]. I [R = α-CH2CH2OP(O)(OH)2, R1 = R3 = tetradecanoyl, R2 = R4 = 4-oxotetradecanoyl, R5 = H] at 100 μg i.v. in mice on the 7th, 12th, and 21st days reducedthe weight of fibrosarcoma tumors in mice to 5% of that of controls.

IT 123598-15-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

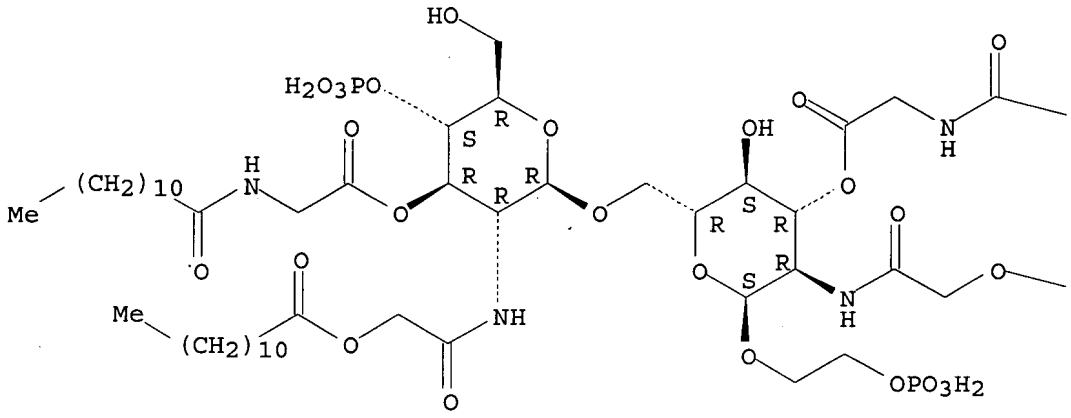
study); PREP (Preparation)
(preparation of, as antitumor agent)

RN 123598-15-2 CAPLUS

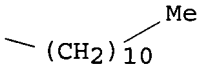
CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-(phosphonooxy)ethyl 2-deoxy-6-O-[2-deoxy-3-O-[[(1-oxododecyl)amino]acetyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-4-O-phosphono-β-D-glucopyranosyl]-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

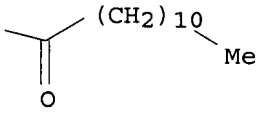
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



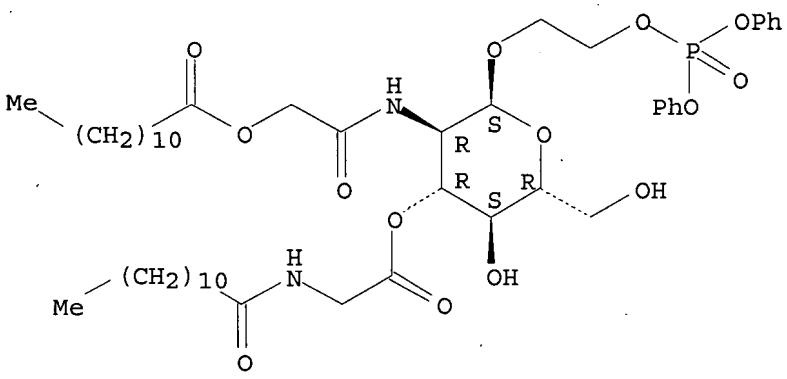


IT 123574-38-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for N,O-acyldiglucosamine phosphate antitumor agent)

RN 123574-38-9 CAPLUS

CN Glycine, N-(1-oxododecyl)-, 3-ester with 2-[(diphenoxyphosphinyl)oxy]ethyl 2-deoxy-2-[[[(1-oxododecyl)oxy]acetyl]amino]-α-D-glucopyranoside (9CI) (CA INDEX NAME)

Absolute stereochemistry.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